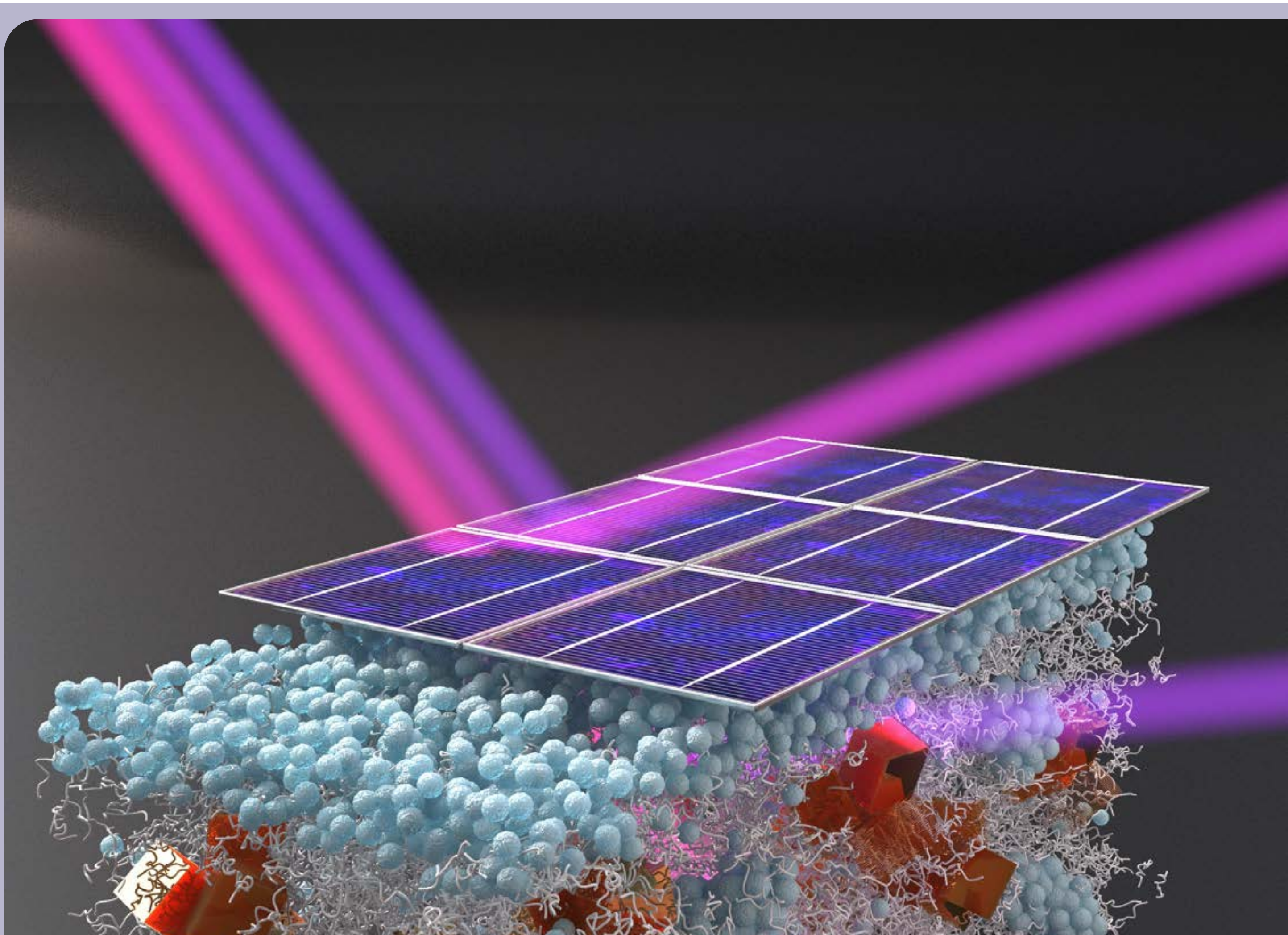
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum



Societal Impact Report

MLZ is a cooperation between:

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technical University of Munich TUM

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Bavarian State Ministry of Science and the Arts

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The Heinz Maier-Leibnitz Zentrum (MLZ):
The Heinz Maier-Leibnitz Zentrum is a leading centre for cutting-edge research with neutrons and positrons. Operating as a user facility, the MLZ offers a unique suite of high-performance neutron scattering instruments. This cooperation involves the Technical University of Munich, the Forschungszentrum Jülich and the Helmholtz-Zentrum Geesthacht. The MLZ is funded by the German Federal Ministry of Education and Research, together with the Bavarian State Ministry of Science and the Arts and the partners of the cooperation.

The Forschungs-Neutronenquelle Heinz-Maier-Leibnitz (FRM II):
The Forschungs-Neutronenquelle Heinz-Maier-Leibnitz provides neutron beams for the scientific experiments at the MLZ. The FRM II is operated by the Technical University of Munich and is funded by the Bavarian State Ministry of Science and the Arts.

Societal Impact Report on the Research Neutron Source Heinz Maier-Leibnitz (FRM II) and its scientific use by the Heinz Maier-Leibnitz Zentrum (MLZ)

A study within the framework of ACCELERATE

ACCELERATE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N. 731112

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Executive Summary

The societal impact of a Research Infrastructure (RI) is manifold, but difficult to quantify. The collaboration with the Rathenau Instituut (The Hague, The Netherlands) within the Horizon 2020 project ACCELERATE enabled us to write this report. Here, societal impact is meant in a broader sense; how does our institute influence the outer world, from the scientific community to the daily life of citizens. It is not a socio-economic report specifying the return of investment based on economic models. This report uses a narrative approach to show our achievements and how we accomplish our mission to provide neutrons for research, industry and medicine. As we do not have a defined model with input parameters, the approval of the impact, to a certain extent, is left to the reader. This report shows and develops narratives based on our goals and mission, the measures to implement our actions and the outcomes achieved. The impact itself on different targets is realised by demonstrating the direct outcome and its importance to related fields. Not all questions associated to an anticipated impact can be answered easily. Is the impact strictly related to the mission and our actions, or did it just happen? Does the impact correspond to the expectations of our stakeholders? Taking into account the wide area of possible impacts, there are rarely simple answers.

The reported narratives span a wide range of views, from the local area of the research campus to its neighbouring city Garching, up to its role in the European Research Area. The basic mission of our research infrastructure is to enable excellent science that can be monitored, using internationally approved key performance indicators based on scientific publications as the final output of experiments performed at the MLZ. It is not only the pure number of publications that impacts the knowledge of a society. New and unexpected results open up entirely new fields in science. Inherent to basic science are the unpredictable results and by this, achievements and impact mainly just happens. Without the availability of our RI, without the continuous funding and effort of our staff in collaboration with our external users, these achievements, however, would have not been possible. Out of this basic research a number of focused investigations are performed at the MLZ addressing key technologies or directly hot topics related to the Grand Challenges of our society. Here the impact to society is more clearly visible as the research questions are more closely linked to the daily life of citizens.

The impact concerning industry and medicine is exercised more strategically. The irradiation of silicon for transmutation doping, the irradiation channels for isotope production and analysis were foreseen right from the beginning of the FRM II and are operated routinely and nearly at the limit of capacity. The worldwide shortage of the isotope Molybdenum-99 for cancer diagnostic pushed us to enlarge the possible isotope production significantly. The impact of these very special products is evident. If we do not produce it, these products would, to a significant extent, simply not be available for our society.

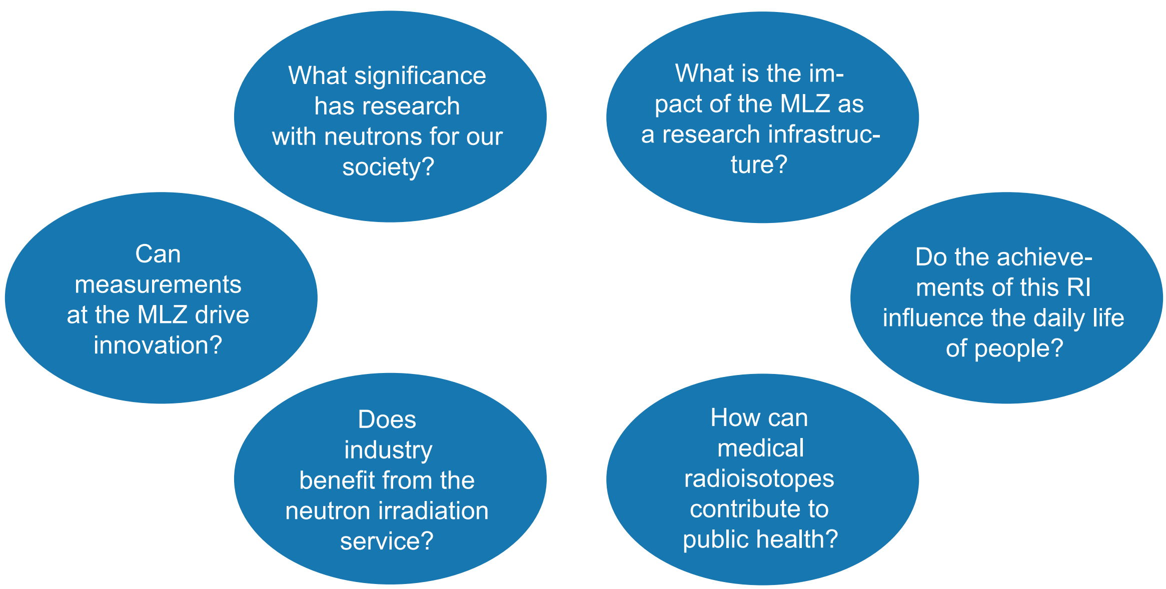
More difficult to trace is the impact of the facility by itself, the relation to local or national economics, the interaction with the general public or the indirect impact by educating highly qualified scientists. Here we have to rely on the judgement of the reader by presenting our concerted efforts in the narratives of this report.


PGAA

Reporting on impact

The Research Neutron Source Heinz Maier-Leibnitz (FRM II), operated by the Technical University of Munich (TUM), acts as a national Large Scale Research Infrastructure (RI) within the MLZ Collaboration enabling the application of neutron beams for the German and international science communities. It also covers industrial research and service in order to achieve optimised usage. Since it started in 2005, a well-documented count of scientific experiments have been processed and, in addition, industry makes use of the irradiation facilities as well as the scientific instruments for applied research. The use of neutrons for medical applications, be it directly through irradiation, or indirectly through the production of radioisotopes for radiopharmaceuticals is well established.

Society might ask numerous questions when it comes to justifying the funding of a research infrastructure by public money. This gave the impetus to collect information for a societal impact report, which sheds light on the contribution to societal welfare.



In this report, you will read about our aim of providing excellence in scientific research, our efforts to supply service for the needs of our industrial customers, and our ambition to address all the questions, the operation of a nuclear installation raises from the public. We will give insight into our plans, how to maintain our impact or even improve it. We will highlight a few examples of our work, which show how fascinating the research and application of neutrons at the MLZ and the FRM II can be.

This societal impact report is carried out within the ACCELERATE (ACCELERATing Europe‘s Leading Research Infrastructures) project. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 731112.

Narrative approach to link science to society

Societal impact is difficult to measure, “first due to the fact that it is indirect rather than direct, and second because it is diffused in space and time” [1]. But what is societal impact of scientific research? This question is addressed not only by ourselves and the project partners of the EU funded H2020-project ACCELERATE in a dedicated work package, but also e.g. as a main scope of the ongoing RI-PATHS (Research Infrastructure Impact Assessment Pathways) project funded by the EU, too. The outcome of RI-PATHS is planned to be an easy-to-use framework for reliable and standardised impact assessments (IA) with the help of a catalogue of questions which an RI can select from, relevant for its situation, and information on the data that needs to be collected to answer them [2]. However, this framework is not in place yet and therefore a selection has to be made out of the wealth of existing approaches and methods used today. For instance, there are journals such as Research Evaluation, Science and Public Policy, Research Policy, and Minerva. In addition, there are consultancy reports dedicated to the societal impact of Research Infrastructures (such as the reports by Technopolis). These reports are often rooted in the same body of academic literature on societal impact and its assessment. Finally, we see the academic literature shine through recent developments in research policy documents dedicated to societal impact of RIs (such as ESFRI [3], OECD [4]). Out of the four broad categories the RI-PATHS project team have defined so far (i.e. direct economic impact, human resource impact, policy impact, and social/societal impact) [2] we chose the latter as the impact area to investigate.

To explain the societal impact of FRM II as a research infrastructure in a broader sense, the authors, together with the experts of the Rathenau Instituut (The Hague, The Netherlands), conducted this study, to demonstrate evidence of impact of daily work in diverse fields such as science, technology, education, economy, culture, society, policy, health and environment. The approach is to take advantage of the “General societal impact protocol – A light on societal impact of ERICs and RIs”, which has been developed in the course of the HORIZON2020 project “ACCELERATE – ACCELERATing Europe‘s Leading Research Infrastructures” by Leonie van Drooge and colleagues of the Rathenau Instituut, especially for this purpose. The protocol suggests a narrative approach, which is now considered best practice [5]. It delivers information on the specific situation and the context of the RI, and the societal impact itself.

A key prerequisite, thereby, is the inclusion of Productive Interactions as defined by Spaapen and van Drooge in their SIAMPI (Social Impact Assessment Methods for research and funding instruments through the study of Productive Interactions) concept [6]. They are defined as ‘exchanges between researchers and stakeholders in which knowledge is produced and valued that is both scientifically robust and socially relevant. […] The interaction is productive when it leads to efforts by stakeholders to somehow use or apply research results. […] Social impacts […] are [then] behavioral changes that happen because of this knowledge’ [7]. Spaapen and van Drooge argue that focusing on ‘productive interactions’ help circumnavigate the time lag and attribution issues commonly associated with outcome-based modes of impact evaluation [6, 8, 9]. They emphasise that assessing the process of impact allows an evaluation which is ‘closer to the actual process that the researcher is able to influence, that is closer to the actual practice of the researcher doing research and interacting with stakeholders’ [8], accompanied by using productive interactions as an indicator which helps anticipate societal impact that may not yet have occurred at the time of evaluation [11]. An overview of alternative impact assessment methods can be found at Bornmann et al. and references therein [10].

Embedded in the needs of funders, scientific users and industrial demands, employees at the MLZ strive to maximise their efforts to enable productive interactions between these and many more stakeholders. They will disclose their intrinsic drivers, which lead them to decisions on how to proceed and develop this renowned RI, the FRM II. You will read, as suggested in [11], a number of narratives, which relate to an impact journey and tell a bigger story of the MLZ and how it has contributed to specific impact.

On the other hand, this is not an evaluation study. We don´t evaluate the impact. However, being part of an “Entrepreneurial University” as TUM calls itself, future developments are considered and inspiration from outside is sought. And there we can learn from e.g. industry, that in taking care of societal impact when setting strategy or adjusting our science model it will reduce the risk of significant negative events and open up valuable new opportunities [12].

[1] B. Godin, C. Doré, Measuring the Impacts of Science; Beyond the Economic Dimension, Urbanisation INRS, Culture et Société. Helsinki, Finland: Helsinki Institute for Science and Technology Studies. http://www.csiic.ca/PDF/Godin_Dore_Impacts.pdf (2005).

[2] RI-PATH, Concept note of modular impact assessment framework. D4.1. https://ri-paths.eu/deliverable/ (2019).

[3] ESFRI Scripta Vol2: Long-Term Sustainability of Research Infrastructures. 94pp., https://www.esfri.eu/sites/default/files/ESFRI_SCRIPTA_SINGLE_PAGE_19102017_0.pdf (2017).

[4] OECD, Main Science and Technology Indicators, Volume 2019 (1), OECD Publishing, Paris, https://doi.org/10.1787/g2g9fb0e-en (2019).

[5] C. Donovan, S. Hanney, The ‘Payback Framework’ explained. Research Evaluation, 20(3), 181–183 (2011).

[6] J. Spaapen, L. van Drooge, Introducing ‘Productive Interactions’ in Social Impact Assessment. Research Evaluation 20, 211–18 (2011).

[7] G. N. Samuel, G. E. Derrick, Societal impact evaluation: Exploring evaluator perceptions of the characterization of impact under the REF2014. Research Evaluation 24, 229–241 (2015).

[8] J. Molas-Gallart, P. Tang, Tracing ‘Productive Interactions’ to Identify Social Impacts: An Example from the Social Sciences, Research Evaluation 20, 219–26 (2011).

[9] S. de Jong et al., Understanding Societal Impact Through Productive Interactions: ICT Research as a Case, Research Evaluation 23, 89–102 (2014).

[10] L. Bornmann et al., Policy documents as sources for measuring societal impact: How often is climate change research mentioned in policy-related documents? Scientometrics 109, 1477-1495 (2016).

[11] L. v. Drooge, J. Deuten, “This large research infrastructure will benefit our region” But how? Eu-SPRI Annual Conference Vienna 2017, 207-210 (2018).

[12] D. Beal et al., Total Societal Impact: A New Lens for Strategy. The Boston Consulting Group. https://media-publications.bcg.com/BCG-Total-Societal-Impact-Oct-2017.pdf (2017).

The FRM II as Large Scale Facility and its regional impacts

The Research Neutron Source Heinz Maier-Leibnitz (FRM II) is operated by the Technical University of Munich and serves as a national Large Scale Research Infrastructure within the MLZ Collaboration. Access to its instruments is based solely on scientific merit. It is unusual in Germany for a RI to be part of a university as the operation of such RI falls to centres of the Helmholtz association and is, therefore, predominantly funded by the Federal Ministry for Education and Research. On the other hand, universities are funded by the local states, and therefore the State of Bavaria has taken over the cost of the construction and ensures the operation of the FRM II. The scientific operation, however, is organised within the MLZ (Heinz Maier-Leibnitz Zentrum) where renowned expert institutes and, consequently different funding resources come together in order to optimise the usage of the FRM II. This special situation implies that the different stakeholders have different expectations and views on the performance and impact of the investments and operational costs. The report on impact starts locally, from the campus in Garching through to a contribution to the European Research Area and on to worldwide collaboration, touching in so many ways on different aspects of society.

The research reactor, inaugurated in 1957, became the nucleus of the Garching research campus. Today, the Garching Research Campus is one of the largest centres for research and education in Germany and Europe.

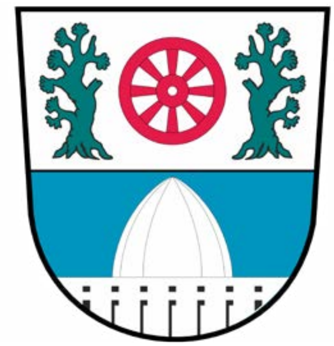
The Garching campus

The scientific campus in Garching was established following the construction of the first research reactor in Germany (FRM, “Atomic Egg”) by the Technical University of Munich (TUM) in 1956 and has since then developed into one of the biggest innovation sites in Europe. In the wake of its foundation, the campus succeeded in attracting the natural science and engineering faculties of the TUM and institutes from the Ludwigs-Maximilians University Munich (LMU). In addition, three institutes from the Max-Planck Society, institutes from the Bavarian Academy of Science including the Leibniz Supercomputing Centre LRZ, the European Southern Observatory ESO, the General Electric Global Research Center Europe and several other research institutes and companies decided to settle here. Today, around 7,500 employees and 17,000 students are working on site at the campus Garching [1].

The ever-evolving campus has significantly affected the public transport infrastructure. The almost 25,000 people that commute every day to the campus prompted the extension of the subway to Garching campus (terminus) in 2006, thereby connecting the city Garching to the centre of Munich. Given that the FRM II operates 24/7, the rail-bound public transport system makes access significantly easier, especially for our users.

Since 1967, the city of Garching has proudly displayed the first German nuclear research reactor in stylised form in the city’s coat of arms. This symbol encapsulates the fact that the Atomic Egg, the nucleus of Garching’s research campus, was associated with progress and faith in the future.

[1] https://www.forschung-garching.de.



Garching Coat of Arms.

The building of the new FRM II

After some 30 years of operation of the FRM, a discussion began as to whether to upgrade or replace the neutron source with a view to regaining an international competitive facility. In1989, the German Council of Science and Humanities (Wissenschaftsrat), who provides advice to the German Federal Government and the State Governments on the structure and development of higher education and research, recommended building a new neutron source in view of the age of the existing sources in Germany. The decision by the Bavarian States Government in 1993 to build the Research Neutron Source in Garching was accompanied by the expectation that major progress would be achieved, especially in the fields of medicine and material sciences. The construction of the FRM II between 1996 and 2004 amounted to an investment of 436 million € in national and regional construction business. This was at the time the largest single investment the TUM had ever made. The FRM II was expected to provide an important locational factor, ensuring future prospects for the Bavarian, German and European research community as well as for the economy [1].

Mayor Helmut Karl receives the certificate that designates Garching a „city“ from Interior Minister Edmund Stoiber in 1990.

Today, the FRM II and the MLZ have a yearly budget of around 60 million €. Together they employ about 400 people on site, including those from collaborating research groups, and host some 1,000 visiting scientists per year who conduct about 1,000 experiments.

[1] Offensive Zukunft Bayern: Regierungserklärung des Bayerischen Ministerpräsidenten Dr. Edmund Stoiber am 21. Juli 1994 im Bayerischen Landtag, 53, 13 S., E. Stoiber (1994).

The development of the University city Garching

In 1956, Garching numbered 2,947 inhabitants. After 60 years, the number of inhabitants had increased six fold to 17,711 citizens (Figure 1), [1]. The village grew with the number of inhabitants. In 1990 the then “municipality Garching” was elevated to the “city Garching”. Only seven years later, Garching was awarded the title “University City” due to the constantly growing Campus Garching. Since 2006, the subway from Munich has been extended, which not only benefits the employees of the Research Campus, but also the population of Garching.

In the last 10 years, the number of TUM-employees at the Garching campus has increased by almost 20%, from 3,079 employees in 2009 to more than 3,630 employees in 2019. About 11% of the TUM-employees at the Garching campus live in the city of Garching [2]. This corresponds to about 2.2% of all inhabitants of Garching. Assuming that 11% of all 7,500 employees from all the various institutes and companies at Campus Garching live in the city of Garching, this would correspond to a share of the population of almost 5%. Many of the other employees live in the communities close by, in Munich or in the peripheral cities of Munich.

Not only the number of employees, but also the number of students has increased tremendously. In the last 30 years, the number of TUM students in total has almost doubled, from 22,864 in the winter semester 1988/89 to 41,375 students in the winter semester 2018/19, [2]. The number of TUM students at Campus Garching has increased almost 8-fold, from 2,071 students in 1988/89 to 16,347 in 2018/19. Two sharp increases are connected to the movement of the Faculty of Mechanical Engineering to Campus Garching in the winter se-

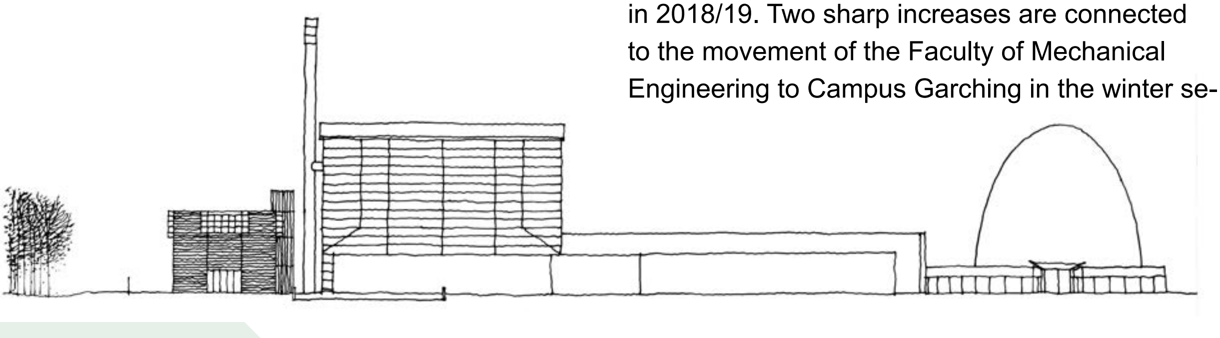
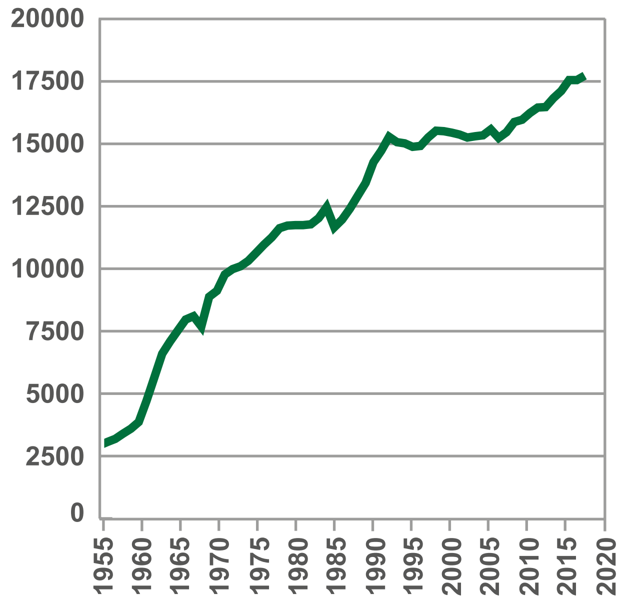


Figure 1: Inhabitants of the city of Garching in the period from 1956 to 2018 [1].



mester 1997/1998 as well as the Faculty of Mathematics and Faculty of Computer Science in the winter semester 2002/2003. Therefore, the TUM benefits enormously from the Campus Garching and its ongoing growth and increasing number of TUM faculties there (Figure 2). All in all, the Atomic Egg, built amongst the cabbage fields of Garching, can be regarded as the seed of a scientific campus that, today, is second to none in Europe.

In a normal year of reactor operation, around 1,000 researchers use the experimental facilities of the MLZ. They are supported by the MLZ User Office which arranges accommodation, about 80% of it being in Garching/Garching Hochbrück and the rest in Munich. Of the approximately 1,351 local hotel rooms available in Garching/Garching Hochbrück, the FRM II/MLZ prefers to make reservations in six hotels offering 475 rooms. In the year 2017 with 3 reactor cycles, 3,055 overnight stays by our users were recorded [3]. Therefore, in a normal year of full operation, users make more than 4,000 overnight stays per year in Garching, which has a direct impact on the economy of Garching.

The Science Congress Centre Munich, built in the middle of the Garching Campus right beside the FRM II/MLZ, will offer further accommodation possibilities in the immediate vicinity for our users and other visitors. Additionally, it will also offer lots of space for conferences, seminars, exhibitions and events for the ever-growing number of students and employees as well as visitors at the research Campus Garching. This new Congress Centre will also make Garching an important venue for international conferences in the light of its infrastructure as well as its bus, train and flight connections.

[1] Bavarian State Statistical Office, Fürth, as of 21.06.2019.

[2] TUM, Hochschulreferat 1 - Controlling, Organisation, Planung.

[3] MLZ Annual Report 2017, p. 89.

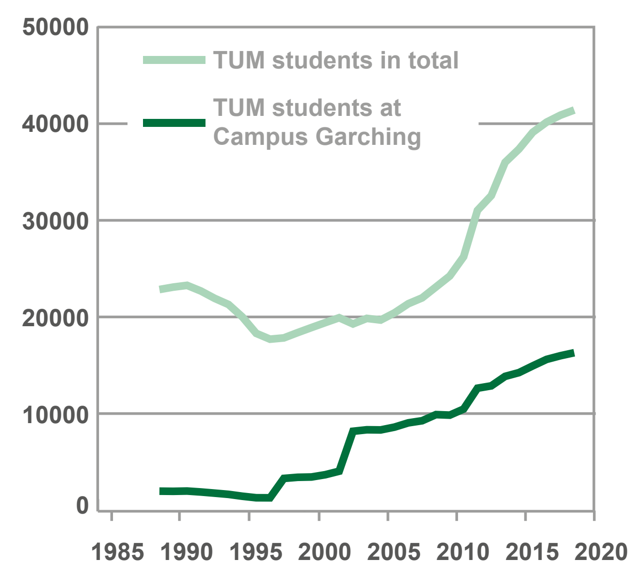
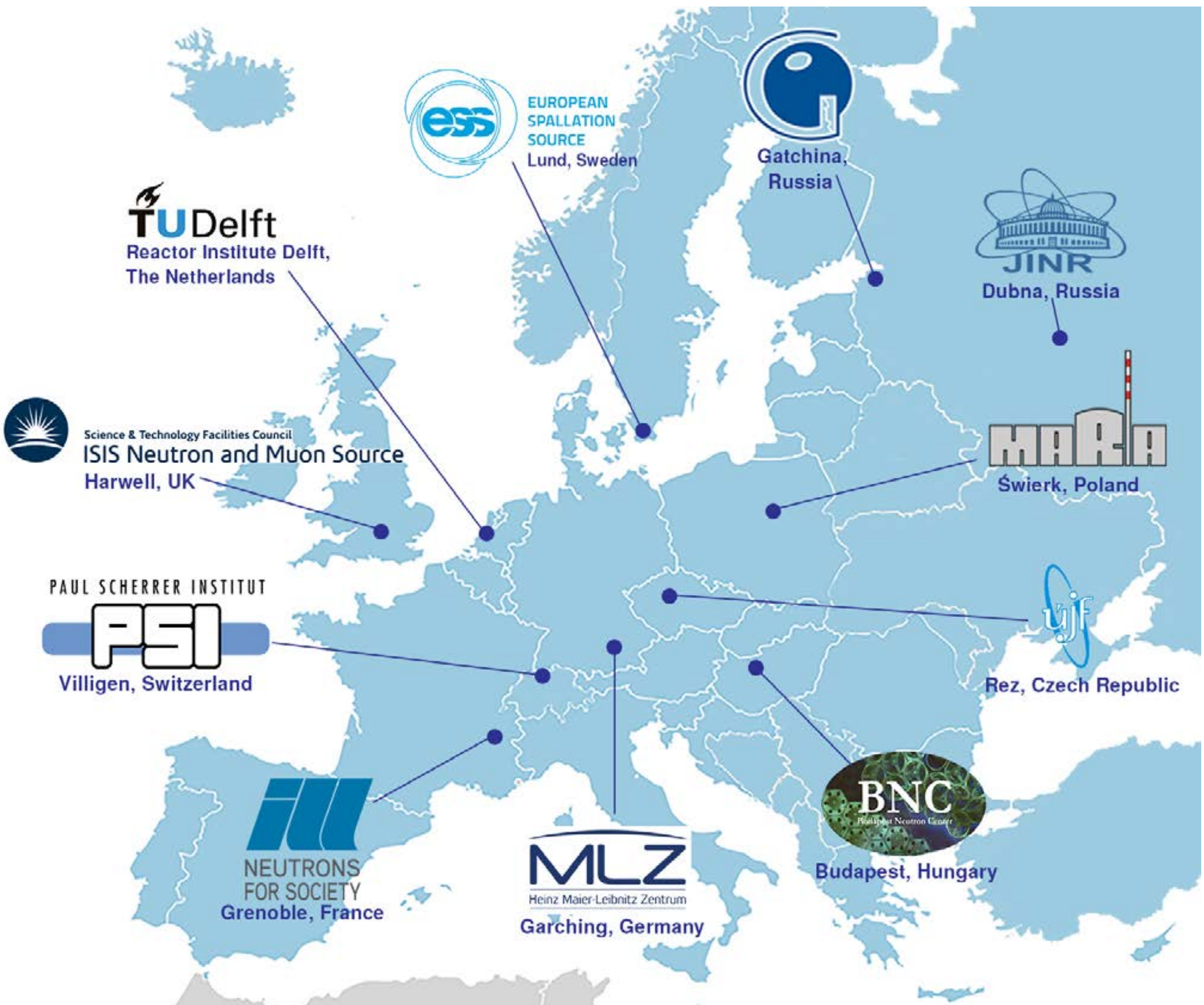


Figure 2: Number of TUM students in total and at Campus Garching during 1989 and 2019 [2].

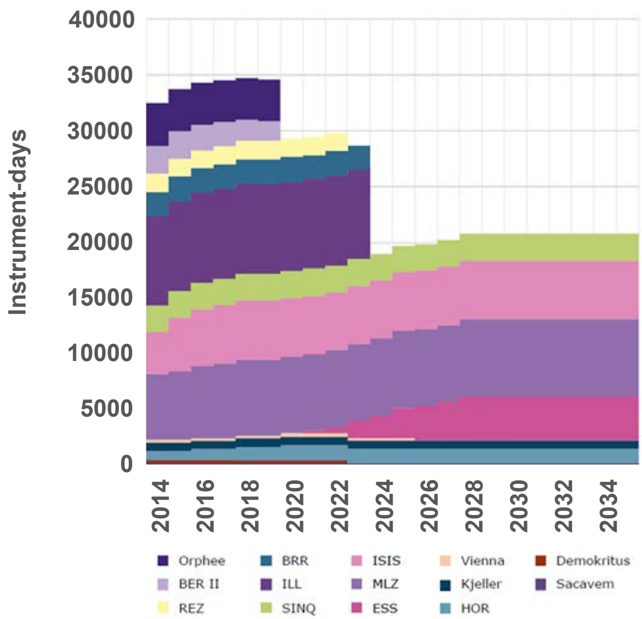
MLZ in the national and international Research Area

On October 31, 1957, the Munich research reactor FRM went online for the first time and produced the first neutrons. In the course of the following years, the „Atomic Egg“ made a name for itself with innovative research work in the fields of chemistry, physics and biology. The scientists developed technologies and standards that were later adopted at other research reactors: Neutron guides, for example, were invented at the Atomic Egg, as was backscattering spectrometry.



Available and future Neutron Research Facilities.

Figure 3: Development of available neutron instrument days in Europe as of 2016 [1].



Based on the pioneering work of Maier-Leibnitz, neutron research began at other facilities in Germany, namely in Karlsruhe, Jülich, Geesthacht and Berlin. In the intervening time, these facilities have been shut down, with the BER II facility in Berlin closing at the end of 2019. With the increased collaboration of the TUM with the Helmholtz Institutes in Jülich, Geeshacht and Berlin, financially supported by the German Ministry for Science and Education (BMBF) and the Bavarian Ministry for Science and the Arts, the MLZ was founded to explore and promote the use of neutron beams for the benefit of the national and international science community. According to the report of the strategic working group of ESRFI (European Strategy Forum on Research Infrastructures), the MLZ plays an increasing role from the point of view of capacity and capability due to the foreseen shutdown of neutron centres in Europe.

[1] ESFRI Scripta Volume I, Neutron scattering facilities in Europe-Present status and future perspectives, September 2016.

Optimising the usage of FRM II by the MLZ

One major goal of the MLZ is to optimise the scientific usage of the neutrons, produced by the research neutron source FRM II. In order to achieve this, we offer an increasing number of high-class instruments to enable state-of-the-art research, promote these instruments to attract high potential users and operate the neutron source as much as possible, up to 240 days a year.

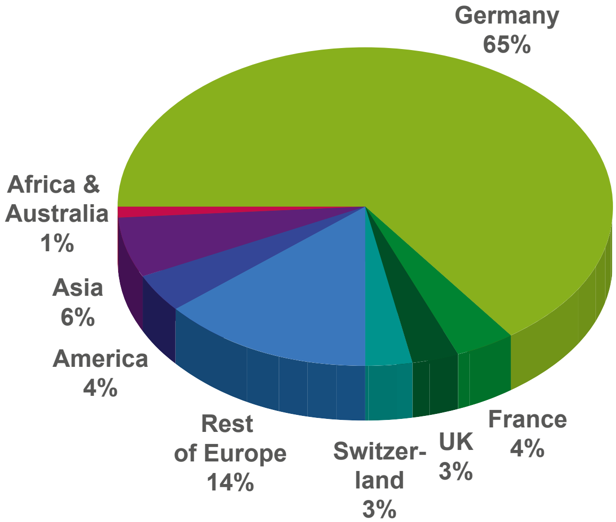
There are now 26 first-class instruments in user operation. More are to come, currently in the construction or planning phase right now. A constantly increasing number of instruments has been achieved through collaboration with German partners, for example the Forschungszentrum Jülich, who transferred 5 instruments from the former research reactor FRJ-2 “DIDO” in Jülich to the FRM II. This was an important step in ensuring the continuation of cutting-edge research with neutrons. The collaboration was further intensified by the signing of a ten-year cooperation contract which will remain in force until 2020. The BMBF, the Bavarian State Ministry of Education, Science and the Arts, three Helmholtz-Centres in Jülich, Geesthacht and Berlin and the Technical University of Munich joined forces to form a world-class neutron scattering centre within Germany which led to the inauguration of the MLZ in 2013.

First-class instrumentation is indispensable to attract excellent users. To ensure the highest quality of performed experiments, and due to the fact that the requested amount of beam time exceeds the time available, the MLZ applies a selection process based on scientific merit. Twice a year submitted proposals are peer-reviewed by an external international referee panel, ensuring high quality criteria and thereby guaranteeing scientific research at the highest level. The allocation of beam time and access to the MLZ is generally free of charge, under the condition that the results are published in a peer-reviewed journal or an equivalent paper and that they are subsequently accessible to the public. The MLZ User Office organises this selection process.

After many successful years of operation, we revised our application process for beam time. The process from application through to performing the measurements may take up to several months. Therefore, in 2013 the MLZ introduced a so-called rapid access program by offering a limited number of beam days for certain instruments via a fast selection process. This access to the instrument enables feasibility studies or sample characterisation prior to the submission of a regular proposal. We began by offering this program for 4 instruments and due to increasing requests from our users, have already increased this number to 9 instruments. To ensure that the rapid access program should not circumvent the usual proposal process, strict criteria for eligibility were established. In order

MLZ scientists at the ECNS 2019 in Saint Petersburg, Russia.

Figure 4: Main proposers' home countries of experiments performed in the years 2011-2018.



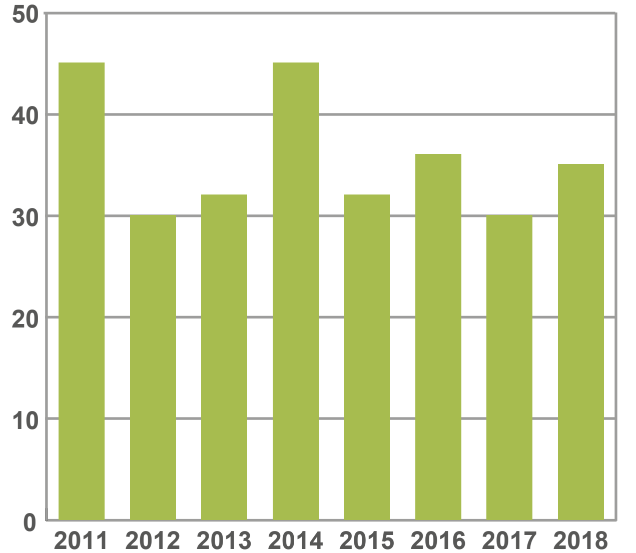
to ensure a qualified selection procedure, in 2018, external referees were engaged for the reviewing process of the rapid access proposals.

Close contact with our users is very important as their demands play a key role in future developments and strategic orientation at the MLZ. Therefore, at the beginning of 2018, we established a MLZ User Committee, consisting of 6 elected international members, representing the MLZ user community. This committee acts as a direct link between our users and the directorate to address new strategic ideas and procedures for continuous improvement of the MLZ users' satisfaction. Furthermore, the MLZ organises regular user meetings and topical conferences to address scientific topics of interest to our users and is represented at various topical conferences such as the conferences on solid-state physics (DPG spring meeting) as well as national, European and International conferences on Neutron Scattering like the German Neutron Scattering Conference (DN), European Conference on Neutron Scattering (ECNS) and International Conference on Neutron Scattering (ICNS), respectively. These activities play a key role in demonstrating the diverse experimental opportunities at the MLZ and getting directly in touch with both our established and potential new users. At the ECNS 2019 in Saint Petersburg, more than 30 scientists from the MLZ out of a total of 572 participants took part, demonstrating the strong contribution of the MLZ to the field of neutron research.

In a normal year of operation, we provide a maximum of 240 beam days, with 4 cycles and 60 days each, for scientific and industrial purposes. Compared to other European neutron sources, this is the highest number of beam days offered so far – the ILL in France delivers around 200 days per year, ISIS in the United Kingdom 120-150 days, the LLB in France 180 days and SINQ/PSI in Switzerland some 190 days. Each year we are able to provide our service for up to 1,000 users, mainly from Germany, but also Europe and even 11% from the rest of the world (Figure 4).

In addition to facilitating excellent science, promoting innovation is a further major objective of the FRM II and the MLZ. Therefore, we offer industry access to our neutron beam instruments to carry out research projects or technical characterisations. If the industrial partner wishes to retain sole ownership of the results, the MLZ offers the possibility of buying beam time under a full cost scheme. Otherwise, the data have to be published as requested for all scientific proposals. A continuous challenge is to find the right balance between industrial and research projects in order to provide sufficient beam time for our users and enable applied innovation-driven research by industry.

Figure 5: Number of journal articles per year dealing with Instrument & Method Development [1].



Development of neutron research at the MLZ as a national hub

Optimising scientific usage of the neutron source FRM II is inherently linked to the goal of attracting the best scientists to perform experiments at our instruments. A prerequisite for this is to offer high performance, uniquely optimised and state-of-the-art instruments and methods. Sustained investment in the development of instruments and methods, including the provision of analysis software, is one of the main criteria for success. A key performance indicator for these investments are results published in peer-reviewed journals on instrument and method development. As indicated in Figure 5, the number of publications by MLZ staff members in this area has been at a high and constant level throughout the last 8 years. It corresponds to about 15% of all articles published by the MLZ. On the one hand, the number of instruments is still increasing and publications on these larger projects have not yet slowed down from the rather high number at the beginning of the routine operation of the FRM II in 2005; on the other hand, upgrades of existing instruments and method development are at a high level with slight fluctuations.

The internationally renowned expertise of MLZ staff members and partners reaches out even to foreign countries. The MLZ partners are involved in the construction of instruments for the new European Spallation Source ESS in Lund, Sweden. This German contribution is the largest of all 18 participating countries and predominantly realised in multi-national cooperation. Of the fifteen instruments currently under construction, seven have a significant contribution from the German partners.

In addition, knowledge of neutron techniques drives a large number of other in-kind contributions on key components for the spallation source itself.

The same consortium of German partners, namely the Helmholtz centres in Jülich and Geesthacht together with the FRM II, aims to support the instrumentation at the PIK reactor in Saint Petersburg within the framework of German-Russian cooperation on large-scale infrastructures. By the end of 2019, the FRM II/MLZ will be the only internationally renowned RI for neutrons in Germany. The concentration of knowledge that incorporates the expertise of a large number of university groups and Max-Planck-Institutes operating instruments at the MLZ in Garching has a strong impact on neutron research in Germany. As a result, the MLZ is likely to become the central hub for neutron methods and innovation for neutron research in Germany, strengthening the leading role of German scientists in this field throughout Europe.

The second factor to make a significant impact on the area of neutron research is education and training. Education in a university curriculum closely linked to research projects is discussed in chapter 7. Here, future scientists are trained in the theory of neutron scattering and expertise is acquired during hands-on courses and using neutron methods in Bachelor, Master and PhD theses. Equally important is the training and education of non-scientific staff, i.e. engineers and technicians. Here, the exchange of knowledge and best practise on an international level is not as evident as in the case of the scientists. To enhance the transfer of knowledge, we have seconded MLZ staff to other national and international neutron laboratories and welcomed even more staff from foreign institutes for internships at the MLZ for up to one year, for instance from the Australian Nuclear Science and Technology Organisation (ANSTO), Australia; China Advanced Research Reactor (CARR), China; Reactor multipropósito RA-10, Argentina and so on. In addition, MLZ staff members participate actively in conferences and workshops dealing with neutron methods and techniques such as the international workshops on sample environment organised by the International Society for Sample Environment, or the annual Design and Engineering of Neutron Instruments Meetings (DENIM), established in 2012.

[1] MLZ publication archive iMPULSE, 2019-04-04.

Participants at the 2014 DENIM workshop organised by the MLZ, Ismaning, Germany.

Impact of the MLZ on scientific disciplines

The Heinz Maier-Leibnitz Zentrum (MLZ) is a leading centre for cutting-edge research using neutrons and positrons. By offering a unique suite of high-performance neutron scattering instruments, scientists are encouraged and enabled to pursue state-of-the-art research in such diverse fields as physics, chemistry, biology, earth sciences, engineering or material science. Our mission is to offer substantial support to scientists from all over the world in addressing the grand challenges facing society today.

In order to fulfil our mission, the selection process for gaining access to our instruments is based solely on the scientific merit of the proposals submitted. No scientific discipline using neutrons or positrons is favoured by our evaluating review panel. On account of this, trends in the application for beam time reflect actual programs by funding organisations and modern research topics. A major condition for using our service is that the results be published in a peer reviewed journal. Consequently, our primary key performance indicator (KPI) is our publication record. The broad variety of different topics addressed by neutron research makes it necessary to introduce a classification scheme which covers all aspects of the topics specified by our users.

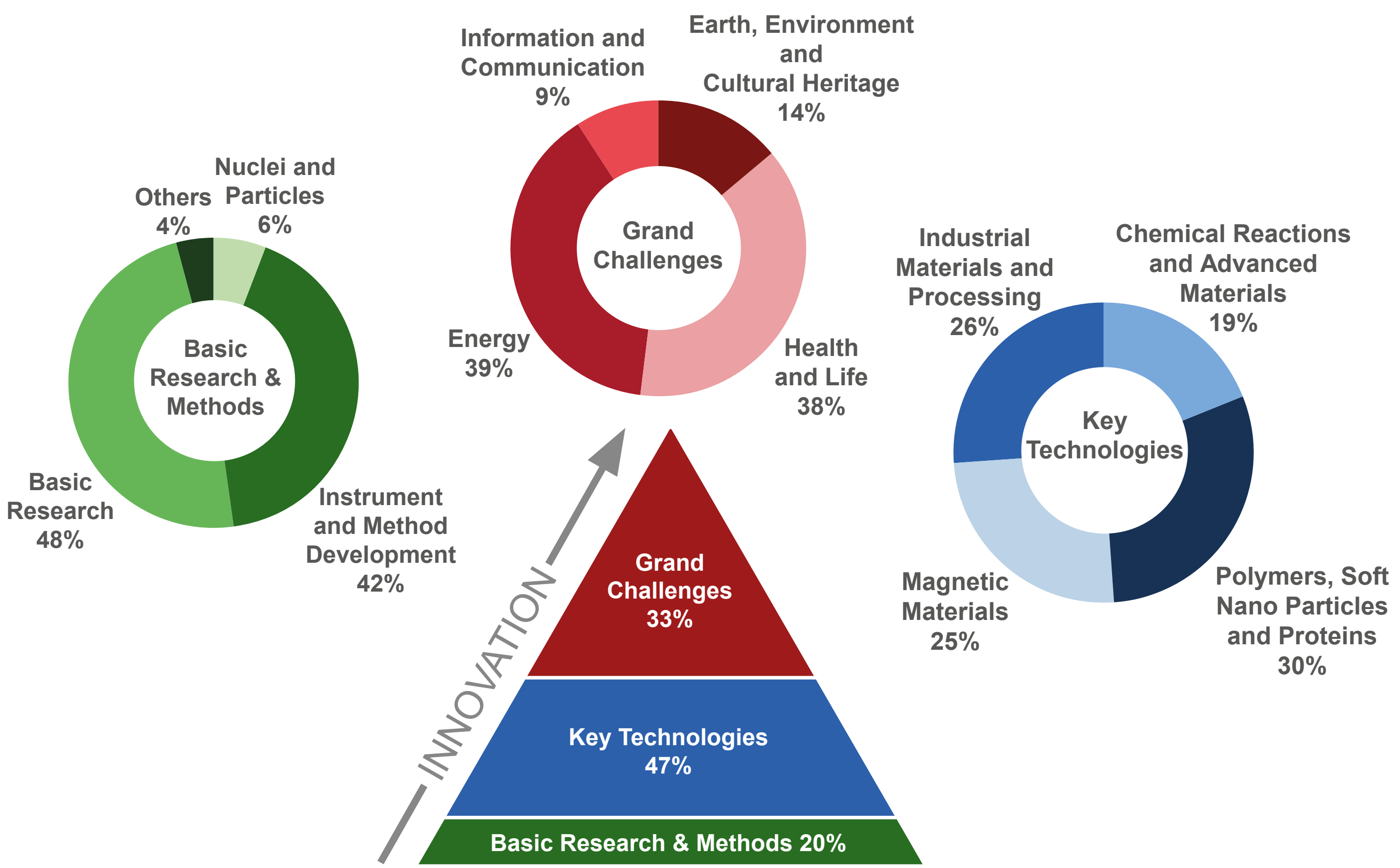
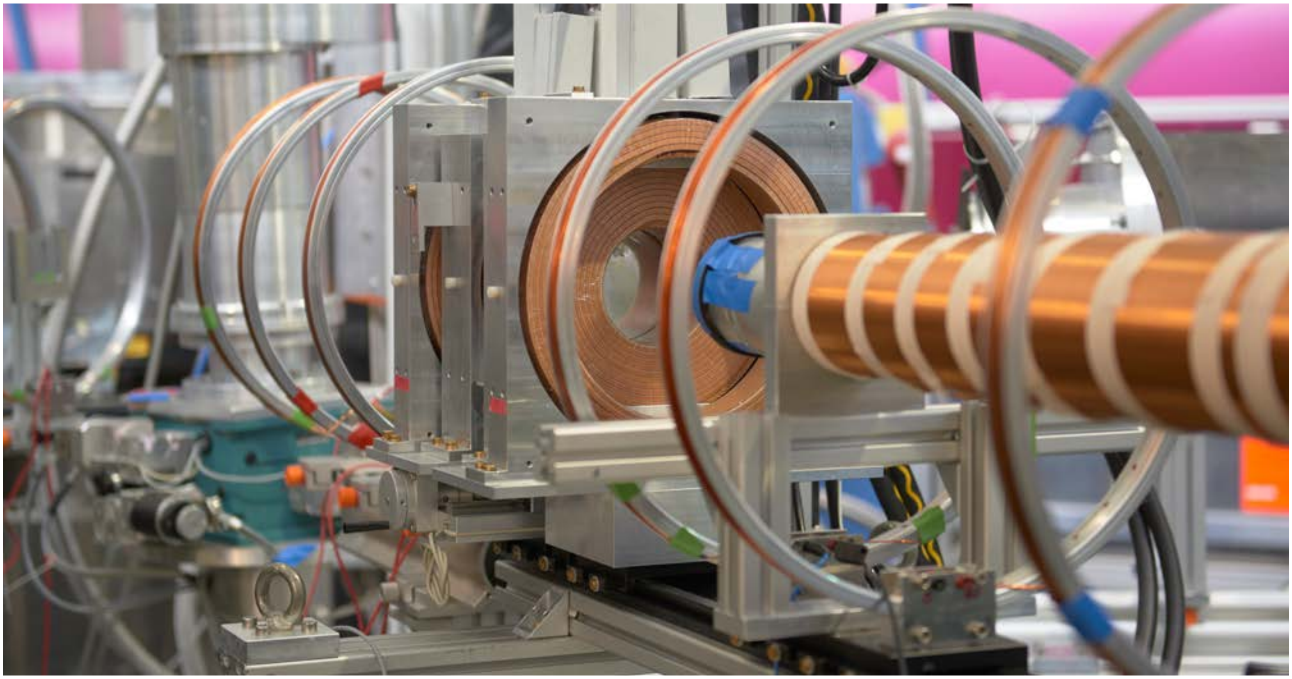


Figure 6: Classification of Journal Articles according to topics 2011-2018 [1].



Instrument RESEDA at the MLZ.

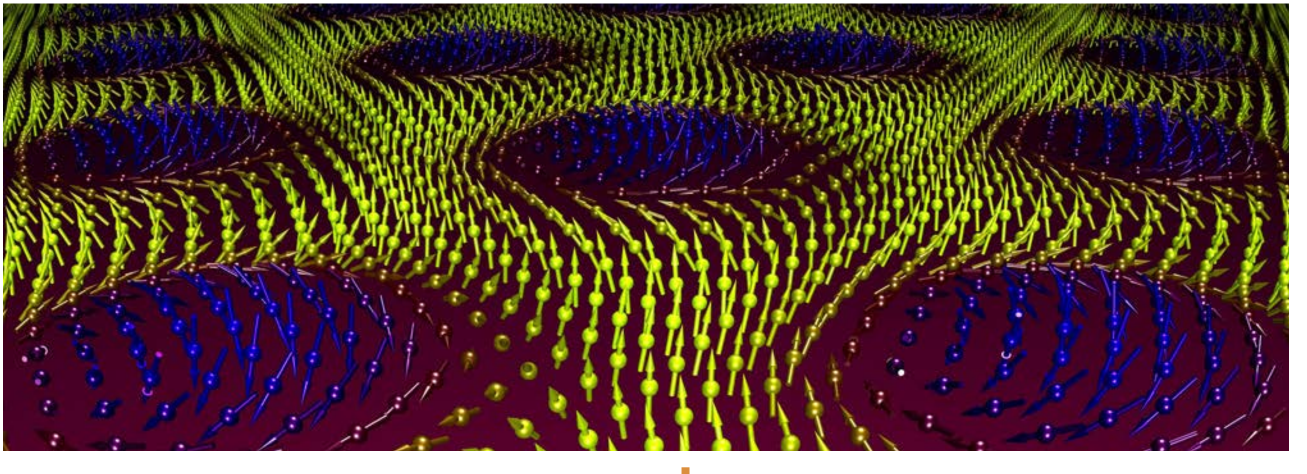
At the MLZ we have developed a scheme with a three-layered structure which reflects the increasing impact of research on society (Figure 6). Basic Research is defined as curiosity driven investigation to explore fundamental interactions between atoms or particles, to understand physical properties and verify new theories. These investigations contribute to general insight in physics or chemistry and establish general laws and rules to understand nature. To this category we added publications of our method and instrument development as this embodies in a similar way the prerequisites for all subsequent investigations using neutrons and positrons.

The second layer, "key technologies", is dominated by the investigation of new materials to understand or discover novel and unexpected properties. The outcome of these experiments is inherently unknown, which is why the impact on society can be neither predicted nor classified. However, research on new materials and hitherto unknown properties is the basis for future development and innovation. We headlined this category "key technologies" accordingly. In order to identify trends and areas in this field, we introduced sub-categories such as "Chemical Reactions and Advanced Materials", "Industrial Materials and Processing" and frequently investigated subjects where neutrons can give unique insight as in the case of "Magnetic Materials" and "Polymers, Soft Nano Particles and Proteins".

Strong evidence for societal impact is given in the third and uppermost layer where research directly addresses the "Grand Challenges" our society is facing today. Grand Challenges, however, can be defined from different viewpoints. We therefore selected headlines which can be addressed via neutron research. This selection of Grand Challenges might be seen as rather specific, but areas of social science such as the Aging Society cannot be meaningfully addressed by the development of new materials. However, in 2015, the United Nations identified key sustainable development goals addressing the most important social, economic, and environmental challenges of our future society. Among the most important goals are affordable and clean energy, health and well-being, industry, innovation, and infrastructure, economic growth, responsible production, clean water, and climate. Tackling these needs denotes the grand challenges for science and technology and leads us to a categorisation of 4 sub-topics, namely Energy, Health and Life, Earth, Environment and Cultural Heritage as well as Information and Communication.

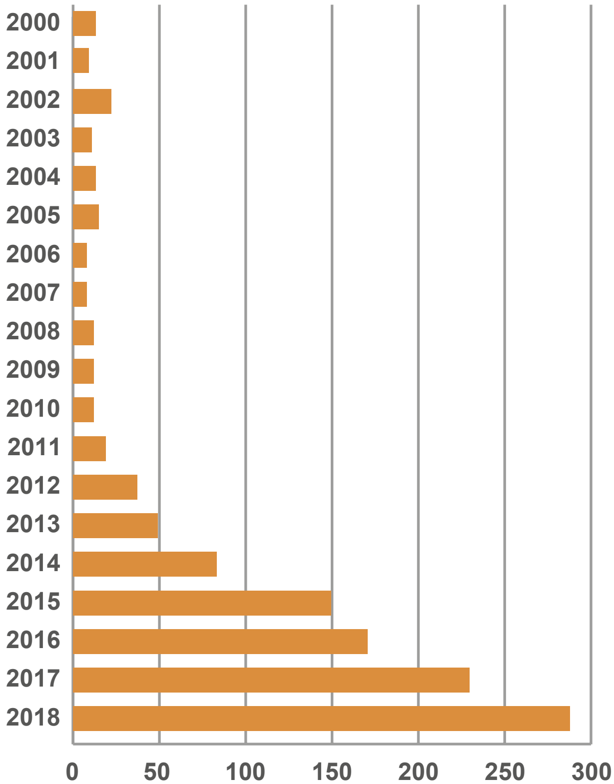
Opening up new research areas

Curiosity-driven research has been a key ingredient for many investigations and many developments that we benefit from today. The MLZ enables fundamental research to simply understand nature and its laws and provides the experimental possibilities to investigate phenomena no-one has as yet discovered. This may open up completely new fields of scientific research. This happened to a team of physicists from the Technical University of Munich (TUM) and the University of Cologne at the MLZ in 2008. They discovered a new type of magnetic ordering phenomenon in the metallic compound manganese silicon, known as magnetic skyrmions [1]. Inspired by a mathematical concept used in high energy physics in the 1960s, a magnetic skyrmion can essentially be seen as a vortex-like structure of the material's magnetisation with a special, non-trivial topology. It is exactly this non-trivial topology that imprints a particle-like character on these tiny magnetic objects. Together with the ease of manipulating skyrmions with remarkably small currents [2], their special vortex-like structure ideally qualifies skyrmions for future



Magnetic ordering on the surface of manganese silicon representing the experimental discovery of skyrmions.

Figure 7: Number of publications dealing with the topic „magnetic skyrmion“ [7].



memory and logical devices that could potentially store information in much higher density than today's data carriers [3].

Inspired by the initial observation at the MLZ using neutron scattering, magnetic skyrmions have in the meantime been identified in a vast number of material classes, even in thin metallic films or nano-structured samples [4, 5]. Skyrmions are no longer limited to cryogenic temperatures; they have even been found well above room temperature. Research on magnetic skyrmions is booming worldwide: The original Science publication of 2009 [1] has meanwhile been cited more than 1,500 times, which ranks this publication amongst the top 0.02% of all scientific publications [6]. From 2000 to 2008 there have been in total 111 papers dealing with magnetic skyrmions and its theoretical prediction. Since its first experimental proof at the MLZ in 2008 and its publication in the Science journal in 2009, the number of papers in that field has increased more than tenfold with about 1,300 publications from 2009 onwards, as depicted in Figure 7.

This discovery of magnetic skyrmions also received recognition through several awards. In 2016, the European Physical Society's prestigious Europhysics Prize was awarded to the experimental physicists Prof. Christian Pfleiderer and Prof. Peter Böni from the physics department of the TUM for the "discovery of a skyrmion phase in manganese silicon", shared with three theoretical physicists: Prof. Alex Bogdanov (Dresden), Prof. Achim Rosch (Cologne) and Prof. Ashvin Vishwanath (Berkeley). Christian Pfleiderer's research on skyrmions had already been recognised in 2012, when he received an ERC (European Research Council) advanced grant, and in 2016 the Max Born prize and medal. Achim Rosch received the Gottfried Wilhelm Leibniz award in 2013, the most prestigious research award in Germany.

The discovery of the magnetic skyrmion lattice is archetypal for the potential impact of fundamental basic research, not only on the scientific community but also on society in general. The transfer of knowledge from fundamental basic research often leads to technical improvements, such as better data storage devices and new logical devices in the case of magnetic skyrmions.

[1] S. Mühlbauer et al., Skyrmion Lattice in a Chiral Magnet, Science 323, 5916 (2009).

[2] F. Jonietz et al., *Spin transfer torques in MnSi at ultralow current densities, Science 330 (6011), 1648-1651 (2010).*
[3] A. Fert et al., *Magnetic skyrmions: advances in physics and potential applications, Nature Reviews Materials 2, 17031 (2017).*
[4] O. Boulle et al., *Room-temperature chiral magnetic skyrmions in ultrathin magnetic nanostructures, Nature Nanotechnology 11, 449–454 (2016).*
[5] S. Heinze et al., *Spontaneous atomic-scale magnetic skyrmion lattice in two dimensions, Nature Physics 7, 713–718 (2011).*
[6] R. van Noorden et al., *The top 100 papers, Nature 514 (2014).*

Scientific publications as a key performance indicator

One important task is to highlight the scientific achievements of the MLZ. The scientific results obtained using MLZ instruments are published in journal articles and are a means of demonstrating the scientific output and accomplishments of the MLZ. Therefore, the number of publications is an important criterion by which to verify the contribution of the MLZ to the advancement of science. The quality of a publication and, hence, its scientific influence is often linked to the so-called impact factor of the academic journal where the scientific articles are published. The impact factor reflects the yearly average number of citations for recent articles published in that journal, with the result that journals with higher impact factors are often deemed to be more important than those with lower ones. Impact factors have been calculated yearly since 1975 for journals listed in the Journal Citation Reports (JCR).

Since 2011, the total number of publications (Figure 8), and the number of articles in prestigious journals in particular, has greatly increased (Figure 9). The grouping of publications with impact factors higher than 7, above and below 1.5 is to a certain extent arbitrary. It provides a means of comparing the scientific output over the years, monitoring the measures taken to improve our performance. Generally, the impact factors vary across all the various scientific fields. Since all audiences are targeted, the data are always published in the journals relevant to the respective scientific disciplines. Many scientific applications at the MLZ are connected, for instance, with materials science as well as instrument and method development. These are of paramount importance for the development of innovative new materials and for high-end instrumentation at the MLZ, but do not usually feature in journals with high impact factors.

[1] MLZ publication archive iMPULSE, 2019-04-04.

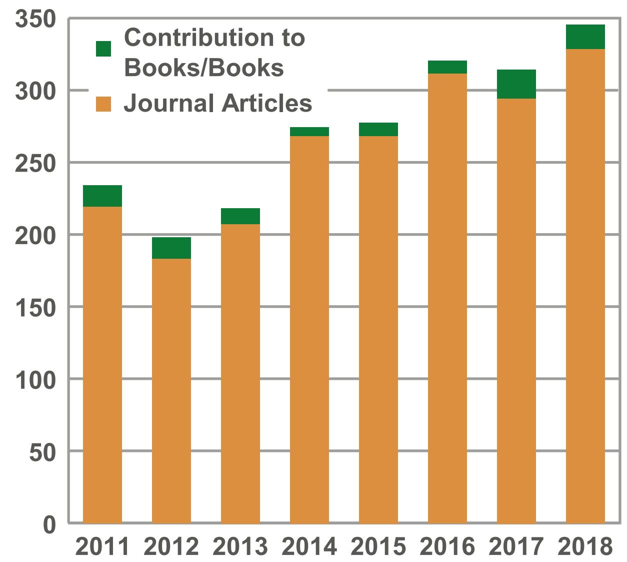
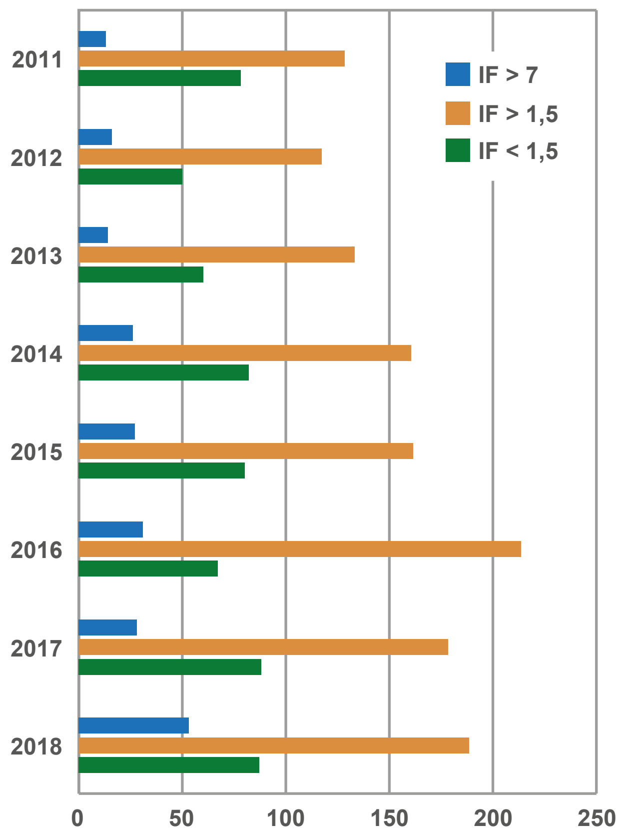


Figure 8: Number of publications, including journal articles and contributions to books [1].

Figure 9: Number of Journal Articles according to Impact Factor (IF) [1].



A further step in innovation and utilisation of the results achieved is envisaged by broadening access to the experimental data our instruments have produced. Within the framework of the German initiative to establish a national research data infrastructure, the MLZ applies for funding within a consortium of RI in Germany, including neutron and synchrotron methods. According to the FAIR principles of the data (Findable, Accessible, Interoperable and Reusable) we generate, we plan to establish the required data infrastructure in order to fulfil these criteria. Allowing access to the data to research groups which did not initially participate in the experiment would ensure that these findings are reused, and in combination with other studies would allow for meta-analysis of experiments. This could lead to entirely new findings, promote the innovation process based on neutron research, and in this way increase even further the impact on society.

Outlook for future improvements and open science

Our mission to facilitate first-class science using neutron and positron beams at the MLZ is based on a network of partners and associated research groups. The close links and exchanges with our scientific users form a sustainable eco-system which impacts strongly on the National and European Research Area. Given continuous funding, sustainability is achieved by a consistently high rate of development and innovation in our instruments and methods. By optimising established methods, we are confident of improving our performance and output constantly.

Contributing to scientific knowledge

With the help of the experimental facilities and support of our own know-how in neutron methods and scientific expertise, we enable basic and applied research to address various questions and goals defined by society and politics. The science accomplished is manifold and touches all areas of life. We have selected some intriguing examples from all layers of the pyramid, from Basic Research, through Key Technologies to the Grand Challenges to give a broad overview of the different fields that are addressed using MLZ instruments. All of them illustrate the use of neutron research to increase scientific knowledge and foster the innovation process.

Information & Communication

Over the past decades, the amount of information stored and processed has witnessed explosive growth. On the atomic level, information processing and storage relates to the manipulation of spin states for which neutrons, due to their spin and related magnetic moment, are uniquely sensitive. Thus, neutrons promote an understanding of the complex correlations of the electronic constituents, which is necessary to develop new materials, increase storage density, create ultra-sensitive sensors for read heads, and to develop new types of computer memory.

A prominent example is the Giant Magnetoresistance (GMR) effect, where a magnetic field influences the electrical resistance. This discovery was awarded the Nobel Prize for Physics in 2007 and is the basis of today's read head technology in magnetic storage media as well as opening up the research field of spintronics based on the manipulation and control of the electronic spin.

Neutrons characterise the microscopic interactions responsible for multiferroics, materials which uniquely combine magnetic, electric and mechanical properties. They are promising candidate materials for sensors and non-volatile, rapid information storage with ultra-small switching capacity. Neutrons characterise the emergence of exotic topological states such as skyrmions which were discovered at MLZ and are being investigated as a basis for new storage devices. Quantum computing and information processing is based on qubits where coupling and entanglement can successfully be investigated via neutron scattering.

Neutrons help to fundamentally understand the emergence of magnetic properties, from the level of the atomic and electronic constituents to the final device function. Neutrons thus serve to develop high density storage devices, low power memory modules, magnetic field sensors and quantum computing, making it possible to store and manage data on smaller scales, as currently observed in smartphones.

A new antiferromagnet enters the scene

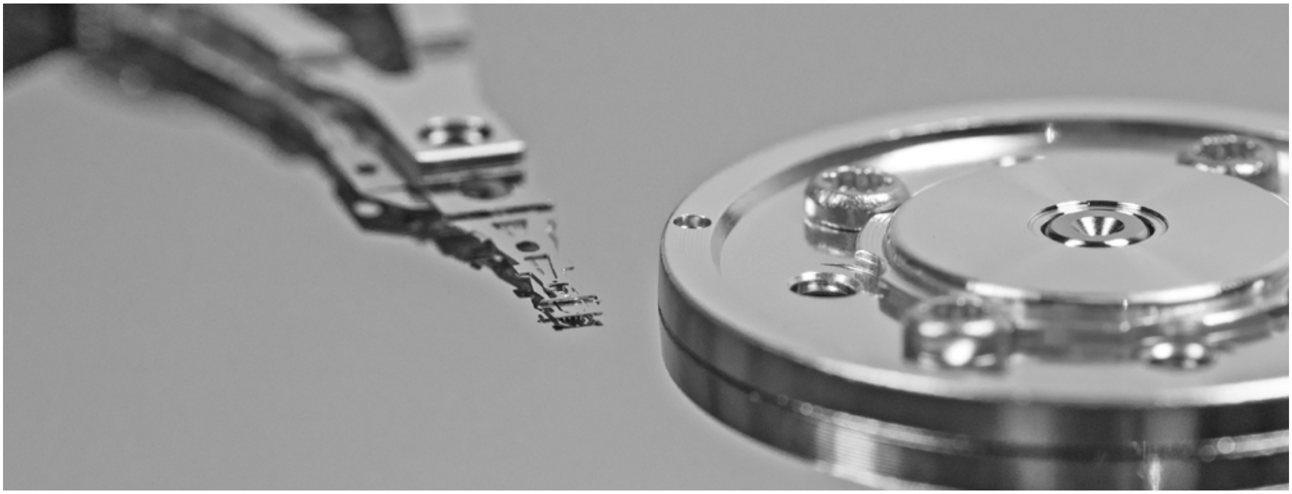
Antiferromagnetic materials have several advantages over conventional ferromagnetic materials. They are insensitive to external and perturbing magnetic fields. Using antiferromagnets in memory devices could help save information more reliably and permanently than ferromagnetic materials can.

A Chinese-German team of researchers has presented a novel synthetic antiferromagnetic material, which may prove pioneering for progress in nanomedicine and information technology. In contrast to a ferromagnet, an antiferromagnet does not show a magnetic field detectable from outside. However, the antiferromagnet is still a magnetic material: It is simply that the little compass needles, “spins”, of the electrons do not point in parallel directions, but are antiparallel. Therefore, the magnetic moments erase each other.

The new synthetic antiferromagnet under study has several ferromagnetic manganese layers only a few nanometres thick, coupled by an ultra-thin isolating titanium oxide layer. This leads to coupled antiferromagnetic spins whose direction of spin changes when they are transferred from one layer to the other. Changes in the layer structure will also alter the properties of the magnetic material. The researchers used polarised neutron reflectivity measurements to show that the single layers of the new material can be magnetised individually. They were also able to show that an external magnetic field can reverse individual layers of the material [1].

[1] B. Chen et al., All-oxide-based synthetic antiferromagnets exhibiting layer-resolved magnetization reversal, Science 357, 191 (2017).

Data could be saved more reliably and permanently using antiferromagnets.



Energy Research

The provision of reliable, clean and sustainable energy sources is one of the fundamental needs of modern societies. Concerns about climate change and the security of our energy supply lead us to harness wind, solar and hydrogen energy and to consider new concepts for future mobility. To address the grand challenges in energy requires the development of new materials for energy conversion, storage, and transport. Neutrons with their sensitivity for light elements, such as hydrogen and lithium, and their large penetration depths provide essential information for energy materials innovations.

Hydrogen is an ideal fuel for our future mobility. Research programmes on hydrogen generation, storage, and power conversion rely heavily on neutron scattering. Materials for electrolysis devices for hydrogen generation, for hydrogen storage and transport, and for fuel cells for power generation are ideally investigated with neutrons. They are an ideal probe as there are particularly sensitive to hydrogen to provide essential information on the movement of hydrogen ions across membranes and their interaction with the electrodes. Lithium is the key material in battery research, for which neutron scattering and imaging are particularly suitable. They provide essential information on the structure, dynamics, and ion-mobility in electrodes, electrolytes, and membranes to improve storage capacity, charge and discharge time, and lifetime.

Solar cells and biofuels provide new and sustainable sources of energy. Flexible and efficient solar cells based on polymers and composite materials offer the potential to harness the abundant energy from the sun. For hybrid solar cells controlling self-organisation and crystallisation is of key importance. Neutrons with their ability of contrast variation play a decisive role in our understanding of the conditions under which these processes take place. The efficient conversion of plants to biofuels requires enzymatic processes, in particular hydrolysis reactions. Here neutron diffraction provides essential information on the protonation states in the active centre of the enzymes, which helps to optimise the enzyme structure for more efficient catalytic reactions.

Neutrons with their large penetration depths are ideal to probe the internal structure of engineering materials that play an essential role in the transport and production of electricity, from steam turbines, rotor blades on wind turbines to materials used in fusion reactors. These structural materials can be well optimised using neutrons.

With the combination of the sensitivity for light elements and large penetration depths neutrons are ideal probes for in-operando experiments. It is possible to observe the lithium distribution in batteries or fuel cells while they are working, or water being produced during the catalytic conversion in a fuel cell while in use. These studies provide valuable information to design energy materials with exceeding performance levels.

Investigation of a lithium-ion battery at the diffractometer STRESS-SPEC.

Life cycle of lithium-ion batteries

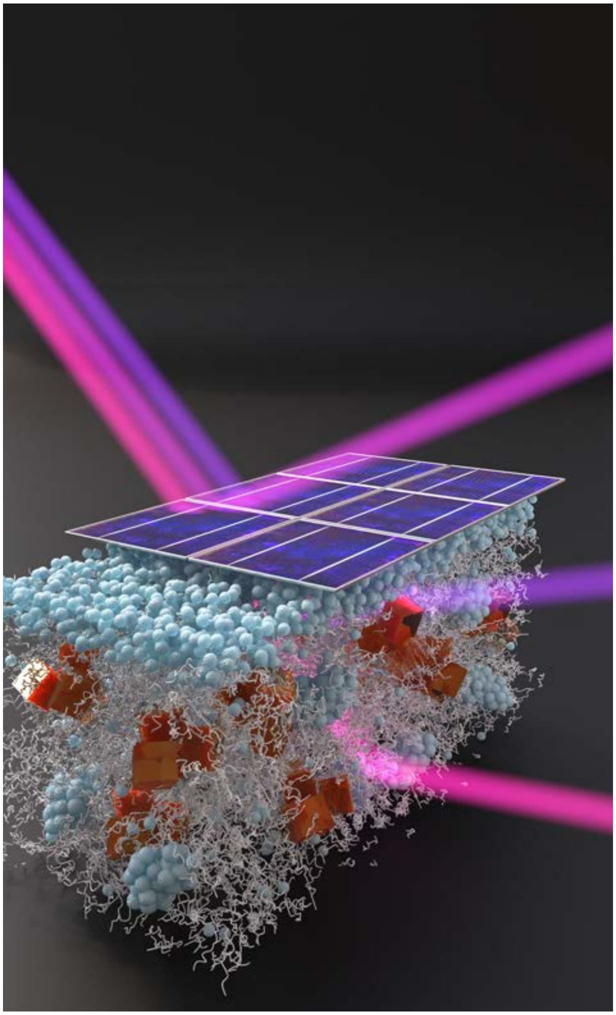
Every day, billions of lithium-ion batteries store electrical charge, relaying it back and forth. Despite the rather simple electro-chemical principle underlying this operation, some background processes affecting battery operation are not yet under complete control, like the loss of capacity upon extensive cycling, safety during charging and discharging or the temperature stability. Neutrons are especially well suited for in operando studies to address these issues, for example on standard size lithium-ion batteries under real operating conditions. Recent spatially-resolved neutron powder diffraction combined with electrochemical measurements and X-ray computed tomography unambiguously revealed variations of the lithium distribution in the graphite anode. Consequently, specific regions in the cells undergo more extensive ion-exchange than others, potentially leading to spatial differences in local fatigue. The spatial profile of Li concentration obtained points directly to the electrical current distribution as a key parameter defining cell performance. Improved use of the applied electrode materials can increase the effective cell capacity and, thus, result in more uniform fatigue and extended cycle life [1].

[1] A. Senyshyn et al., Homogeneity of lithium distribution in cylinder-type Li-ion batteries, Scientific Reports 5, 18380 (2015).

Neutrons to achieve higher efficiency of solar cells

Organic solar cells consist mainly of hydrocarbon compounds. Consequently, their production can be significantly cheaper using printing processes than conventional photovoltaic cells based on silicon technology. Major development goals cover the long term stability and to raise the performance of transforming light into electrical energy.
So far efficiencies up to 13% are achieved when converting solar into electrical energy. Neutrons are the tool of choice for looking deeper into the inner morphology of organic solar cells, especially to develop new materials for further optimisations. One development branch deals with the supplement of additives to the light transforming hydrocarbon compound like the solvent additive 1,8-octanedithiol (ODT). An increase of the efficiency is expected by modifying the internal structures of the solar cell. The researchers [1] added various concentrations of ODT, analysing them with grazing incidence small angle neutron scattering at the instrument REFSANS.

The results showed that the surface and the interior of an intermediate layer were similar in a cell without the additive ODT and that some isolated nano-islands had formed. Charge carriers, important for the functioning of a solar cell were trapped in these islands. Adding ODT, the structure of the solar cell is quite different: there are fewer traps, the interconnections are much better developed and, by this, charge carriers can be transported more efficiently. However, neutrons also showed that there is a limit beyond which an additional additive does not increase efficiency



Organic solar cells consist of hydrocarbon compounds.

anymore. The ODT induces a compact layer of acceptors on the surface which as a consequence lowers the efficiency significantly.

[1] W. Wang et al., Influence of Solvent Additive 1,8-Octanedithiol on P3HT:PCBM Solar Cells, Advanced Functional Materials, 1800209 (2018).

Health & Life

The understanding of the essential processes of life requires knowledge of how biomolecules such as proteins, DNA and membranes perform their roles. This basic knowledge provides insights for the development of improved drugs and biomaterials for diagnostics and therapy in medicine. The ability of neutron scattering with its sensitivity to light elements allows accurate determination of the molecular structure and dynamics of biomolecules, which is essential to better understand the properties of biomolecules in general.

In particular, neutrons help to improve drugs and biomedical materials. Examples include studies of the interactions of drugs with biological membranes and target molecules, the optimisation of shape memory implant materials, and the improvement of biomaterials for surgical procedures. To understand the molecular causes of diseases, neutrons provide important structural and kinetic information e.g. on amyloid aggregation, relevant in the early stages of neurodegenerative diseases such as Alzheimer's, or on cholesterol transport with effects on neurodegenerative and heart diseases.

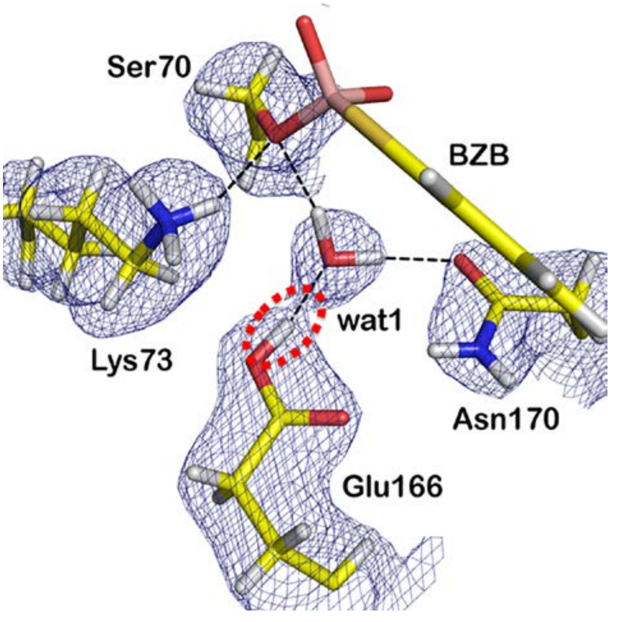
Neutrons also provide important insights into fundamental bimolecular processes. With their sensitivity for hydrogen and the possibility to highlight parts of biomolecules by deuteration (exchange of hydrogen atoms by its chemically equivalent isotope deuterium), neutrons are able to provide insights into protein structure and show details of the protonation states in the active centres of enzymes. Neutrons address key questions such as how charge is moved across membranes, how water is oxidised to oxygen photosynthetically, how metabolic charge transfer reactions are catalysed, and how surface interactions cause proteins to fold in particular ways. Furthermore, neutrons are useful in unravelling the role of the dynamics of biophysical processes, such as allostery and functional dynamics in enzymes, or the movement and function of proteins in crowded environments, such as in the cytosol.

Neutrons reveal mechanism of bacterial antibiotic resistance

More and more bacteria are becoming resistant to antibiotics. They achieve this, for example, by hydrolysis of the β-lactam ring in penicillin and related antibiotics, thus making these drugs useless. It is still not fully understood how the enzyme beta-lactamase in bacteria carries out this process. Some important details of the reaction mechanism are still controversial. However, the understanding of this mechanism could help develop new antibiotics. Leighton Coates and co-workers from the Oak Ridge National Laboratory, USA, have now studied in detail the mechanism of a β-lactamase enzyme using neutrons at the MLZ.

They used the diffractometer BioDiff, which is optimised to study the atomic structure of proteins. In order to locate the hydrogen atoms in the enzyme using neutron diffraction, the researchers replaced all hydrogen atoms in the enzyme by its heavier isotope, the deuterium atom. Thus, the positions of the deuterium atoms in the active site of the enzyme could be determined, while the enzyme is bound to an antibiotics' analogue.

During the reaction in the active site, a proton acceptor temporarily takes a proton. So far there have been two conflicting hypotheses about which residue acts as the general base in part of the mechanism. Numerous studies have suggested it is the Lys-73 residue, while other studies suggested the Glu-166 residue. The neutron scattering experiments at BioDiff, complemented by high-resolution X-ray analysis, however, clearly showed that the Glu-166 acts as a proton acceptor [1].



Result of the neutron structure analysis shown as a blue mesh and the resulting structure model. The red circle highlights the hydrogen atom (white) of Glu166.

[1] S. J. Tomanicek et al., Neutron and X-ray Crystal Structures of a Perdeuterated Enzyme Inhibitor Complex Reveal the Catalytic Proton Network of the Toho-1 β-Lactamase for the Acylation Reaction, Journal of Biological Chemistry, 288(7):4715-4722 (2013).

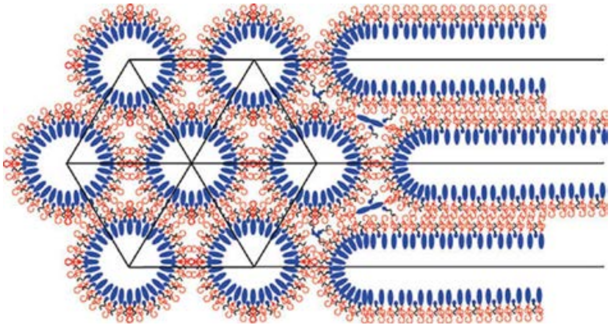
Neutrons provide new explanations for side effects of Ibuprofen

Ibuprofen is an active substance often used in the treatment of pain, fever and inflammation. However, if taken over a long period of time, certain risks present themselves, such as dangerous gastric bleeding. How this rare side effect develops on a molecular level has not yet been explained. Using a model system, researchers from the Jülich Centre of Neutron Science and from the Ludwig-Maximilians-Universität München have now shown that high doses of Ibuprofen can change the structure of lipid membranes. These types of membranes form the walls of healthy cells; the structural changes observed would be toxic for cells.

The scientists were able to detect these structural changes using a model system of phospholipids from soy plants with the help of neutron scattering techniques using the instruments MARIA and J-NSE at the MLZ. At low concentrations of Ibuprofen, the lipids examined formed parallel bilayers, which is usual for the cytomembrane of healthy cells. At high concentrations however, the membranes exhibited an ordered structure made up of holes.

The concentrations studied are far in excess of the estimated levels in medical applications. Researchers find it conceivable that shortly after taking the medication, high concentrations may occur temporarily in certain places and – one might assume – this could be enough to cause tiny defects in the cell walls. Further studies should reveal whether this type of structural change can actually be observed in lipids of animal origin with complex structures [1].

Ibuprofen (represented by the small blue circles with black "tails") lodges itself in layers of lipids (large blue ellipses with red tails). High concentrations lead to the formation of patterns made up of pores (left); at low concentrations, lipid bilayers can be found (right).



[1] S. Jaksch et al., Influence of Ibuprofen on phospholipid membranes, Physical Review E 91, 022716 (2015).

Earth, Environment & Cultural Heritage

The understanding of environmental and earth sciences is crucial to help us finding solutions to the problems that arise from ongoing global change. Population growth, increasing urbanisation, the growing demand placed on natural resources, industrialisation, environmental pollution, greenhouse gases and associated climate change and the natural disasters this sometimes provokes, all challenge our environment and our standard of living. Research can help us understand processes taking place on earth and evaluate outcomes, consequences and the impact of human activities. This can eventually provide the driving force to foster political action for the establishment of a sustainable future, such as expanding clean technologies.

However, it is not only the gaining of more in-depth knowledge about our present and future which is important, but also the investigation of our past. The precise and non-destructive investigation of archaeological discoveries is of great interest.

Neutrons are an invaluable tool to non-invasively analyse precious fossils, ancient artefacts, and works of art. They are non-destructive, can penetrate deep into cultural artefacts or beneath the surface of paintings and are sensitive to isotope composition to reveal microscopic structures, chemical composition, and to provide 3D images of the inner parts. The origins and history of objects from museums and archaeological sites can be safely investigated using neutron scattering without damaging them or affecting their value. Museum experts are able to decipher the methods used by artists and craftsmen by detecting details of the microstructure and composition of the artefacts. Pigments in paints and glasses can be investigated to detect forgeries. Neutrons help conservation programmes for buildings and sculptures by assessing porosity, corrosion, erosion, or the migration of water into materials. Neutrons thus provide valuable and complementary information to address questions of provenance, authenticity, fabrication techniques, and conservation.
In all three fields of geosciences, environment, and cultural heritage, we can gain new knowledge by employing the diverse analytical methods available to us using neutrons.

A prophet's head on the Florence Gates of Paradise was examined at the PGAA instrument at the MLZ.

Cirri, the ice clouds in the upper troposphere (8-12 km high) look like teased cotton wool.

Looking inside ice clouds

Ice clouds in the lower stratosphere (15-20 km altitude) play an important role in the radiation balance of our planet, exerting a strong influence on the climate, or on ozone depletion at the polar caps. The particles inside these clouds consist primarily of water ice and nitric acid trihydrate (NAT): the latter can assume either an alpha- or beta-form. Researchers from TU Vienna, supported by scientists from the MLZ, focused on the alpha form of the hydrate, which is only temporarily stable. Using the powder diffractometer SPODI, they were the first to fully understand the structure of this alpha-NAT. Since the beta-hydrate is present in the atmosphere at the end of the ice cloud formation, they also studied the phase transition and found the beta form with a similar volume, but a more symmetric structure than the alpha. This was the first proof of the independent existence of the alpha-NAT. As long as enough ice is available, the alpha is always produced first. This metastable form only exists between -85°C and -73°C if the alpha crystals are in contact with ice and slowly changes into the beta form. It has a high affinity to water ice, which plays a crucial role when it comes to the formation of ice clouds [1].

[1] F. Weiss et al., Metastable Nitric Acid Trihydrate in Ice Clouds, Angewandte Chemie International Edition 55, 3276 (2016).

Safer underground storage of carbon dioxide

The underground long-term storage of carbon dioxide (carbon capturing and storage, CCS) is anticipated to contribute to the reduction of the emission of climate-changing gases in the atmosphere. The storage of CO_2 in porous rock layers deep underground is so far the favoured solution. This storage of anthropogenic CO_2 in geological formations relies on a cap rock as the primary seal preventing the introduced super-critical CO_2 from escaping. Although natural CO_2 reservoirs demonstrate that CO_2 may be stored safely for millions of years, uncertainty remains in predicting how cap rocks will react with CO_2-bearing salt water. This uncertainty poses a significant challenge to the risk assessment of geological carbon storage. In the case of a natural reservoir in Utah, USA, current experiments have found the top layer to be stable for at least 100,000 years, or ten times as long as calculated by current models. An international research team investigated the pore network structure of a natural carbon dioxide reservoir in Utah by means of small angle neutron scattering at the KWS-1 and KWS-3 instruments. The investigations described the diffusivity and reactions of the carbon dioxide dissolved in water and showed that the CO_2 remains stored in certain types of cap rock layers far longer than first envisaged [1].

[1] N. Kampman et al., Observational evidence confirms modelling of the long-term integrity of CO_2-reservoir caprocks, Nature Communications 7, 12268 (2016).

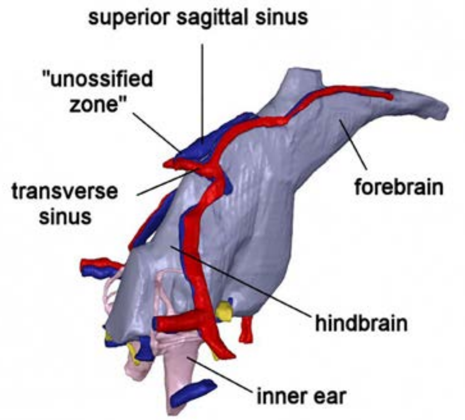
The rocks in the Colorado Plateau, USA, are representative of reservoirs currently under consideration for CO_2 storage.

Mystery of an enigmatic impression in the braincase solved

For more than 100 years, palaeontologists have speculated about the possible function of the so-called “unossified zone”, which is an unossified space on the inner side of the skull roof at the level of the hindbrain of the mammalian ancestors, the therapsids. However, a wide range of interpretations exist. For example, it has been hypothesised that parts of the hindbrain occupied this cavity, that it was a functionless space in the skull roof or the cast of a blood-filled chamber. Now, researchers from the University of Duisburg-Essen could shed light on the function of this enigmatic brain cavity. In collaboration with scientists from the MLZ they investigated a fossil skull of a 255 million year old therapsid Diictodon feliceps by means of neutron tomography using the instrument ANTARES. Further measurements using neutron radiography were conducted at the Paul Scherrer Institute in Switzerland for comparison.

Due to the high penetration depth of neutrons, neutron radiography is well suited to investigate internal cranial structures of fossil skulls. In contrast to X-rays, which often will be absorbed by the iron-rich matrix of the fossils, neutrons are well suited to penetrate them and produce a good contrast between bones and surrounding matrix material. As a result, more than 800 tomographic slices generated by neutron tomography revealed the presence of several canals of blood vessels, which terminated in the unossified zone of the tetrapod vertebrate’s body length. Diictodon was a member of the extinct herbivorous group of dicynodonts.

Until now, very little is known about the shape of the therapsid brain and its blood supply because



3D Reconstruction of the brain endocast of Diictodon feliceps showing the unossified zone and the reconstructed blood vessels (red/dark blue).

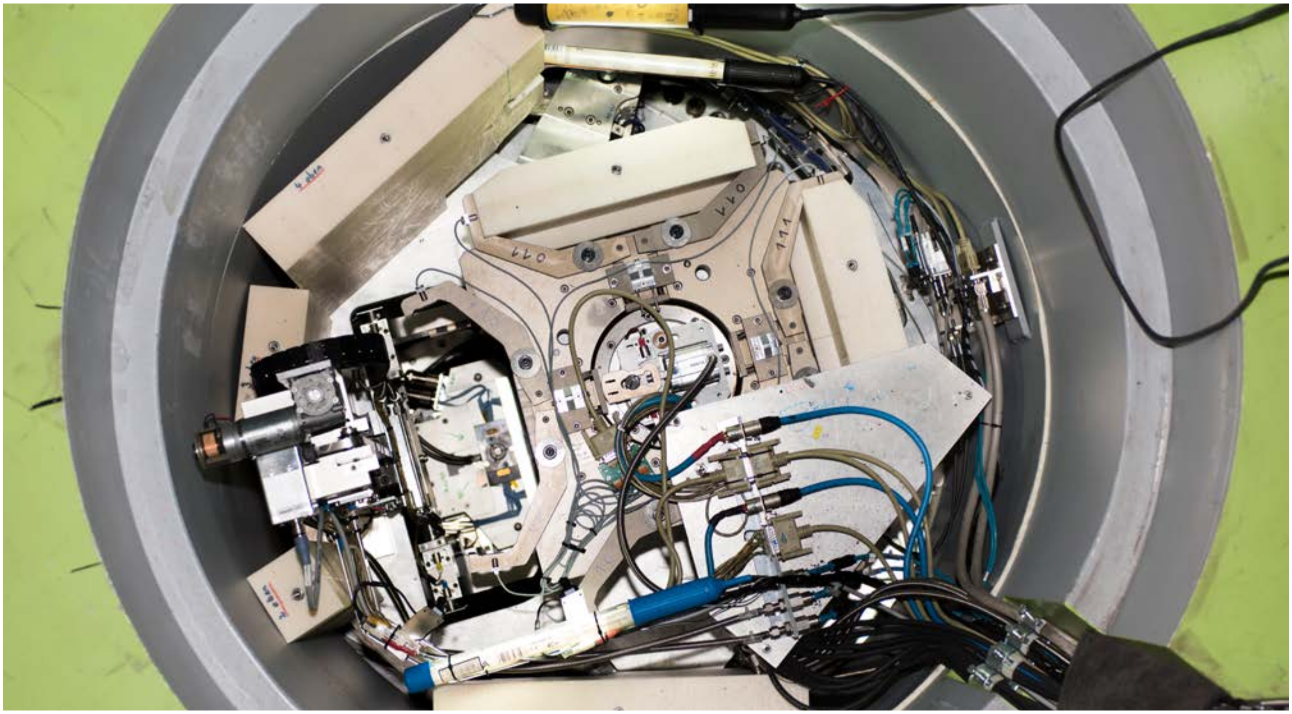
soft tissue is not preserved. As a consequence, information about the shape of the therapsid brain can only be deduced from the surrounding brain cavity. Unfortunately, the brain cavities of most therapsids were only incompletely ossified and preserved. Moreover, it seems likely that the brains of therapsids did not often fully occupy the braincase, similar to modern turtles and reptiles today. A further problem might be that blood vessels were often covered by the meninges.

The neutron measurements showed that Diictodon´s brain was obviously in close contact with the surrounding bones. Therefore, the brain and several blood vessels left sharp impressions in the braincase. These results enabled the scientists to make a less hypothetical reconstruction of the brain, and its system of blood vessels, of our far relatives [1].

[1] M. Laaß et al., What did the “Unossified zone” of the non-mammalian therapsid braincase house? Journal of Morphology 278(8), 13 p. (2017).

Magnetic Materials

Technologies based on quantum physics already account for more than a quarter of the gross domestic product of modern industrial societies. Examples are magnetic resonance tomography and X-ray radiography in medicine, photovoltaic plants in energy technology, and semiconductor devices in information and communication technologies. A current focus is on quantum phenomena such as magnetism or superconductivity. The transfer and storage of energy without any significant loss is a great challenge when developing new materials, such as high Tc compounds in energy technology. It would lead to new materials with lower heat loss and better electrical conduction. Although the mechanism of high-temperature superconductivity is still not completely understood, neutrons have contributed significantly to our basic understanding by shedding light on the interaction between superconductivity and magnetism as well as superconductivity and lattice vibrations.



The three-axes-spectrometer PANDA showed, how the magnetic resonance of the material developed.

Exploring the origin of high-temperature superconductivity

Since the discovery of high temperature superconductivity, researchers have tried to find out why these materials already become superconducting at comparatively high temperatures. They all show neutron spin resonance, which is a collective magnetic excitation that appears in the unconventional copper oxide, iron pnictide and heavy fermion superconductors below the critical temperature. But what is the reason for this behaviour? Inelastic neutron scattering at PANDA turned out to be a convenient method for studying this resonance behaviour, and showing how the magnetic resonance of the material develops and acts at the critical point where superconductivity occurs. In most common superconductors, magnetism suppresses superconductivity. An international team compared the neutron scattering data with theoretical calculations of the electronic structure and the results from scanning tunnelling microscopy. In this study they were able to show that, to the contrary, it seems that magnetic fluctuations resembling those in ordered magnets appear to be essential for the appearance of superconductivity in this class of materials [1].

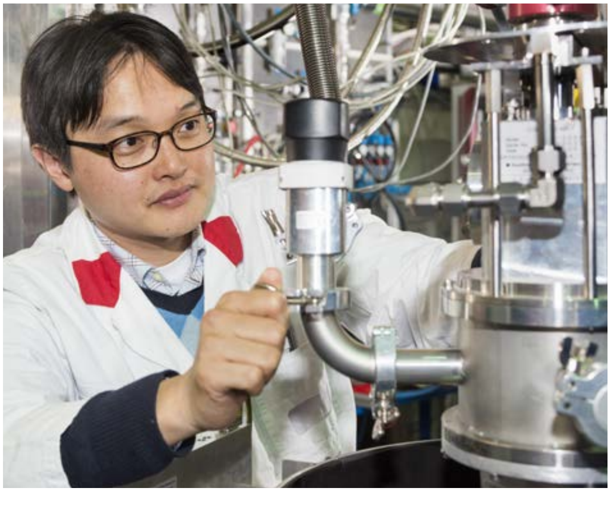
[1] Y. Song et al., Robust upward dispersion of the neutron spin resonance in the heavy fermion superconductor $Ce_{1-x}Yb_xCoIn_5$*, Nature Communications 7, 12774 (2016).*

Unconventional superconductors

Transporting electricity without losses is the promise of superconducting materials. Iron-based superconductors are a complete mystery for researchers as iron is actually a magnetic material, which should prevent the superconductivity. Electrons can be visualised as tiny compass needles and all are in parallel in magnetised iron. However, for conventional superconductivity, the electrons must be coupled antiparallel with spherical symmetry (phase preserved order) for the formation of the superconducting Cooper pairs. This seems to be different with iron-based superconductors. Therefore, they are also named “unconventional superconductors”.

Neutrons scattered from an unconventional superconductor often carry the information about the structure of the superconducting electron pair (Cooper pair). Here, researchers always observed a peculiar excitation of spins in the iron-containing superconductors briefly below the transition temperature at which the material becomes superconducting. This so-called magnetic resonant mode indicates a phase reversed alignment of the electron compass needles, supporting the idea that the spin excitations are a sort of “glue” for the Cooper pairs.

Preparation for an experiment at the instrument PUMA.



Using the three-axes spectrometer PUMA, the two scientific teams from Japan and China (Advanced Industrial Science and Technology and Fudan University), in collaboration with scientists from the MLZ, observed a transition from phase-reversed to phase-preserved Cooper pair formation. This reversal of the signs obviously depends on the degree of doping of the iron-selenide and iron-arsenide superconductors under investigation. If the superconductor had more than 50% sulphur in the iron-selenides and 80% of potassium in the iron-arsenides added, the mode suddenly disappears, indicating that the electron pairs changed back to phase-preserved symmetry. The findings suggest that the iron-based superconductors are much more complicated than previously thought, which retains their interest as an ongoing research topic [1-2].

[1] C. H. Lee et al., Suppression of spin-exciton state in hole overdoped iron-based superconductors, Scientific Reports 6, 23424 (2016).
[2] Q. Wang et al., Transition from Sign-reversed to Sign-preserved Cooper-pairing Symmetry in Sulfur-doped Iron Selenide Superconductors, Physical Review Letters 116, 197004 (2016).

Industrial Materials & Processing

Materials science and engineering are key elements in the development of new technologies and innovation. In order to optimise materials, processes and components, neutrons provide detailed insights into their structure and dynamic properties. Due to their high penetration depths for metals and ceramics, together with their isotope sensitivity, neutrons are a unique diagnostic tool. They contribute to materials development from the atomic scale to the visualisation of complete engines over several orders of magnitude in length scales. This helps to improve performance and is of relevance for the ageing and failure of materials. Neutrons help to tailor alloys at the atomic level or confirm the cause of structural failure after major accidents. Neutrons penetrate deep within materials and are at the same time sensitive to (especially light) atoms. This makes it possible to observe and optimise the behaviour of lubricants in engines while they are running.

For construction materials, such as those required in the aircraft industry, overcoming internal stresses in materials is of key importance. Airbus, for example, replaces rivets with welded seams in its new aircraft. As internal stresses accumulate and are exacerbated on exposure to external pressures, it is extremely important to successfully manage material stress to ensure the safety of the aircraft. Neutrons are routinely used to validate the welding processes. In aircraft construction, lightweight components mean a reduction in fuel consumption. An example here is the optimisation of aluminium/silicon-multiphase materials. Their strength comes from the precise control of the casting process as well as the careful monitoring of the solidifying process. In-situ neutron experiments with high intensity neutron beams widen our knowledge base significantly.

Neutrons provide valuable information from the atomic level to the performance of the bulk material. This leads to the development of lightweight high-strength materials, used to make cars and aircraft lighter, skyscrapers stronger, and laptop cases stiffer.

Tensions cast in steel

Stresses in metals lead to deformations and, in the worst case, to cracks in the material when used in components under mechanical load. Such residual stresses mainly affect work pieces made of two different metals, such as cylinder liners in car engines. The metals, which are placed around each other like rings, expand differently during cooling after casting. This creates tension between the two materials. Uwe Wasmuth from TUM has used neutrons at the MLZ to investigate such a composite mould in situ during cooling.

These results, obtained during his PhD at the chair of Metal Forming and Casting at the Technical University of Munich is also inspiring industry. He was able to show that a commonly used computer program that simulates the stresses in work pieces made of two metals does not take an important factor into account. The program calculated the stresses three times higher than they actually were. The simulation ignores the fact that the aluminium ring in the test cylinder still adapts slightly to the harder and less shrinking steel core through creep processes.

The stresses were determined on a work piece consisting of two aluminium and steel alloys used in industry at the STRESS-SPEC instrument at the MLZ. He poured the 710°C hot aluminium around the already finished steel core. The strain was determined in-situ during cooling by measuring the atomic distances and thus allowed conclusions to be drawn about the stress in the entire work piece. With the help of STRESS-SPEC it was observed that stresses corresponding to a load of up to 20 kilograms per square millimetre only occurred at a

In-situ casting of an aluminum block at the instrument STRESS-SPEC.

cooling temperature of 350°C or higher. The aluminium contracts twice as much as the steel when it cools. These enormous forces are only visible by a few hundredths of a millimetre around which the steel sleeve deforms during cooling [1].

Repeated presentation of the results of these neutron measurements to the foundry industry introduced great interest in finding a generalised computer model for the creep process, which weakens the stresses between the metals. Only precise computer simulations that also take temperature-dependent creep processes into account can accurately predict the stresses in work pieces and thus prevent cracks.

[1] U. Wasmuth et al., Optimisation of composite castings by means of neutron measurements, CIRP Annals 57 (1), 579-582 (2008).

New super-alloys for energy conversion

The efficiency of gas turbines is closely related to a high working temperature and this limits the materials that can be used for turbine blades. State-of-the-art nickel base super-alloys cannot tolerate higher temperatures, even when coated by a ceramic protection layer. A new alloy has been studied which contains cobalt and rhenium to achieve an improved heat-resistance and high mechanical strength. Cobalt itself can withstand high forces, is known in turbine construction and would be a favourable basic material, but can only be used in the medium temperature range. Rhenium itself can withstand extreme high temperatures up to 3000°C. Altogether, there are eight different components of the new alloy, especially tantalum carbides and chromium. Chromium protects the material against corrosion or oxidation and tantalum carbides increase the strength. In a simplified manner, such an alloy consists of a matrix in which fine nanoscale precipitates, here the tantalum carbides, are incorporated for stabilisation.

So far, alloys are mainly characterised under the microscope, before and after heat treatment at high temperatures. With neutrons, in-situ investigations during heat treatment are possible. In addition, neutrons can be used to observe the size, shape, and distance of the stabilising precipitates during the heating phase. For the investigation of the Co-Re alloys five different instruments and methods were used at the MLZ.

In-situ neutron experiments at high temperatures and load.

The investigation has already yielded valuable information to the material developers on exactly how long and at which temperature the heat treatment has to be conducted to optimise the alloy. However, at very high temperatures above 1300°C, the microstructure becomes unstable and the material becomes brittle. So far the new Co-Re alloy is long-term stable up to 1200°C, whereas the nickel-base alloys can only be used up to 1100°C. For a gas turbine this would mean that the combustion is cleaner, and a higher efficiency by up to a few percent can be achieved. However, it will take at least 15 years from now to be applied. And there are other ideas for the use of the alloy, e.g. for materials in rocket engines [1-3].

[1] R. Gilles et al., Stability of TaC precipitates in a Co–Re-based alloy being developed for ultra-high-temperature applications. Journal of Applied Crystallography 49, 1253–1265 (2016).

[2] L. Karge et al., The influence of C/Ta ratio on TaC precipitates in Co-Re base alloys investigated by small-angle neutron scattering. Acta Materialia 132, 354-366 (2017).

[3] D. Mukherji et al., Neutron and synchrotron probes in the development of Co-Re-based alloys for next generation gas turbines with an emphasis on the influence of boron additives. Journal of Applied Crystallography 47, 1417-1430 (2014).

Polymers, Soft Nano Particles & Proteins

Materials and products relevant for our daily life comprise soaps, detergents, paints, and personal care products as well as industrial scale emulsions for tertiary oil recovery, lubricants to reduce friction, membranes for separation and purification, foams for foods, and polymers for light-weight materials. These are often complex, hierarchically structured multi-component materials or formulations consisting mostly of light elements. Here neutrons can provide essential knowledge on molecular to macroscopic length, time and energy scales that is essential to improve their performance.

Soft materials play a key role in many of the grand challenges for sustainable energy, i.e. membranes for fuel cells, batteries, and electrolysers, active layers for solar cells, improved health and safety, i.e. drug carriers, shape-memory materials, and membranes for water purification, protection of our environment, i.e. porous media for carbon sequestration, and transport and mobility, i.e. new lubricants, fuel additives, bio-inspired light-weight and self-healing materials.

Further examples include smart responsive materials that react in a controlled way to outside stimuli such as stress, temperature, pH, and electric and magnetic fields to transduce force, release drugs or trigger enzyme activity. Neutrons are essential for characterising structures and interfaces at the nano- and mesoscale in nanocomposites, biomimetic materials and microemulsions. The ability of contrast variation to highlight specific molecular parts or components are an indispensable tool to decipher the structure of single components as well as their motion.

Many molecules spontaneously form nanoscale assemblies that can form hierarchical structures useful for drug delivery, multifunctional nanocomposites, and high-performance membranes. Nano- and mesoscale materials are structured over a large range of length scales, for which neutrons can provide essential information. Formulation and processing of these materials often leads to non-equilibrium states with unusual structure and properties. Neutrons are particularly suited for related in-situ studies of the structural and dynamic response of soft materials under external stress as well as external electric and magnetic fields.

Neutrons also are essential for the development of new catalysts for more efficient energy use, for reduced environmental pollution, and new chemical synthesis for pharmaceuticals, fuels, plastics, and fertilisers. Neutrons allow the study of active catalysts during operation. Researchers can follow the individual steps of a catalytic process to optimise and tailor catalyst structure. Transient chemical species that form during the reaction can be identified by studying how their characteristic vibrations change, often involving hydrogen, for which neutrons are particularly sensitive.

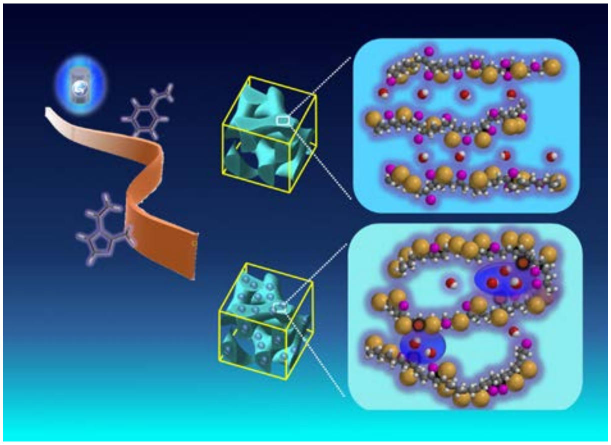
Improved membranes for platinum-free fuel cells

Fuel cells have great potential to reduce our dependence on fossil fuels and the air pollution this brings, thus lessening the impact on climate change. Jülich scientists at MLZ, together with colleagues from Japan, have discovered how fuel cell membranes can be improved without the use of rare and expensive precious metals such as platinum.

Fuel cells using anion exchange membranes instead of proton-exchange membranes, can do without acid-resistant precious metals. Their electrodes consist of inexpensive, non-precious metal catalysts. However, their performance and long-term stability are not yet sufficient, despite major advances over the past decade in developing new materials and optimising system design. The biggest difficulty is that the very properties that make the membranes so efficient have up to now simultaneously reduced their long-term stability. For the first time, researchers from Jülich and Japan have succeeded in producing and characterising membranes in which this correlation appears to have been overcome.

The membranes presented in this study were produced by Japanese researchers working at the car manufacturer Daihatsu and the National Institute for Quantum and Radiological Science and Technology (QST) in Takasaki using one of several common methods: graft polymerisation. In the process, they, to a certain extent, implanted areas in the membrane with different properties. For the grafting, they used hydroxide-conducting and water-repellent units in various mixing ratios. At first they were surprised to see that more hydrophobic and fewer hydrophilic grafts led to higher water uptake, and therefore to increased alkaline degradation, and vice versa. The neutron scattering studies at the instrument KWS-2 also showed that the membrane's lifespan increased when it had more hydroxide-conducting and fewer hydrophobic grafts, causing the water regions to be homogeneously distributed. In order to design new ion-exchange membranes, not only their composition but also their microstructure should be taken into consideration, along with the distribution of the ionic groups and the water in the conducting regions. The German-Japanese research team has therefore proposed a model that, for the first time, can quantitatively explain the distribution of the graft polymers in either the conducting or non-conducting phase. It can be applied to all functional graft polymer membranes.

[1] K. Yoshimura, et al., Reverse relationships of water uptake and alkaline durability with hydrophilicity of imidazolium-based grafted anion-exchange membranes, Soft Matter, 2018, 14, 9118.



Anion-exchange membranes with hydrophilic graft copolymers being alkaline stable (top right) and membranes with hydrophobic graft copolymers undergoing alkaline degradation (below).

Lifetime of magnetic spin waves in antiferromagnets understood for the first time

Using high resolution neutron scattering at the instrument TRISP of the Max-Planck Society at the Heinz Maier-Leibnitz Zentrum (MLZ), the lifetime of magnetic spin waves was measured and, for the first time, a correct theory was developed. The aim of the study, which was published in Physical Review Letters [1] was to understand the lifetime of magnetic spin waves in simple models of anti-ferromagnets. In contrast to the known ferromagnets like iron, the magnetic moments of neighbouring atoms are each oriented in the opposite direction.

The spin waves of the magnetic moments only live for a few nano seconds, thus the waves are dampened. This lifetime is a prerequisite to understand many material properties. For the first time, this was measured using high resolution neutron scattering of the instrument TRISP at the MLZ. The results show that hitherto existing theories have predicted incorrect lifetimes. Using the data of the measurements at TRISP, Alan Tennent of Helmholtz-Zentrum Berlin could develop a new theory. This will also enable the calculation of lifetimes in other materials.

Many new materials, like high temperature superconductors or quantum magnets, are anti-ferromagnets. The magnetic spin waves are fundamental for the function of these materials, and key to understanding the appearance of superconductivity. The measurements at the MLZ will contribute significantly to further understanding.

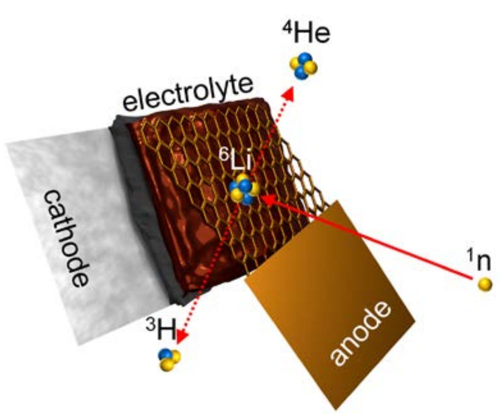
Neutron-resonance-spin-echo setup at the TRISP instrument.

[1] S. P. Bayrakci et al., Lifetimes of Antiferromagnetic Magnons in Two and Three Dimensions: Experiment, Theory, and Numerics, Physical Review Letters 111, 017204 (2013).

New methods made available for battery research

In the last years, lithium ion batteries have spread widely, in particular in mobile applications and in the electro-mobility sector. New concepts and materials need to be characterised in order to increase the efficiency and their lifespan. Neutron Depth Profiling (NDP) is developed and implemented as a new method at the MLZ. It makes use of the high neutron capture capability of specific nuclei like lithium, which subsequently decay into two charged particles where their respective energies are well defined. Since charged particles lose energy when traveling through matter, one can determine the depth of their origin by measuring their residual energy when leaving the sample. This allows for the precise determination of their distribution in the sample.

As Lithium-6 is well suited for this method, it is particularly powerful for lithium-ion-battery research. Using this method ex situ measurements are possible, where electrodes are removed from batteries after charging or after different numbers of charge-discharge cycles. Additionally, the method also allows for operando measurements where the whole battery can be analysed.



Lithium captures a neutron and by this scientists can determine the location in depth of the lithium atom.

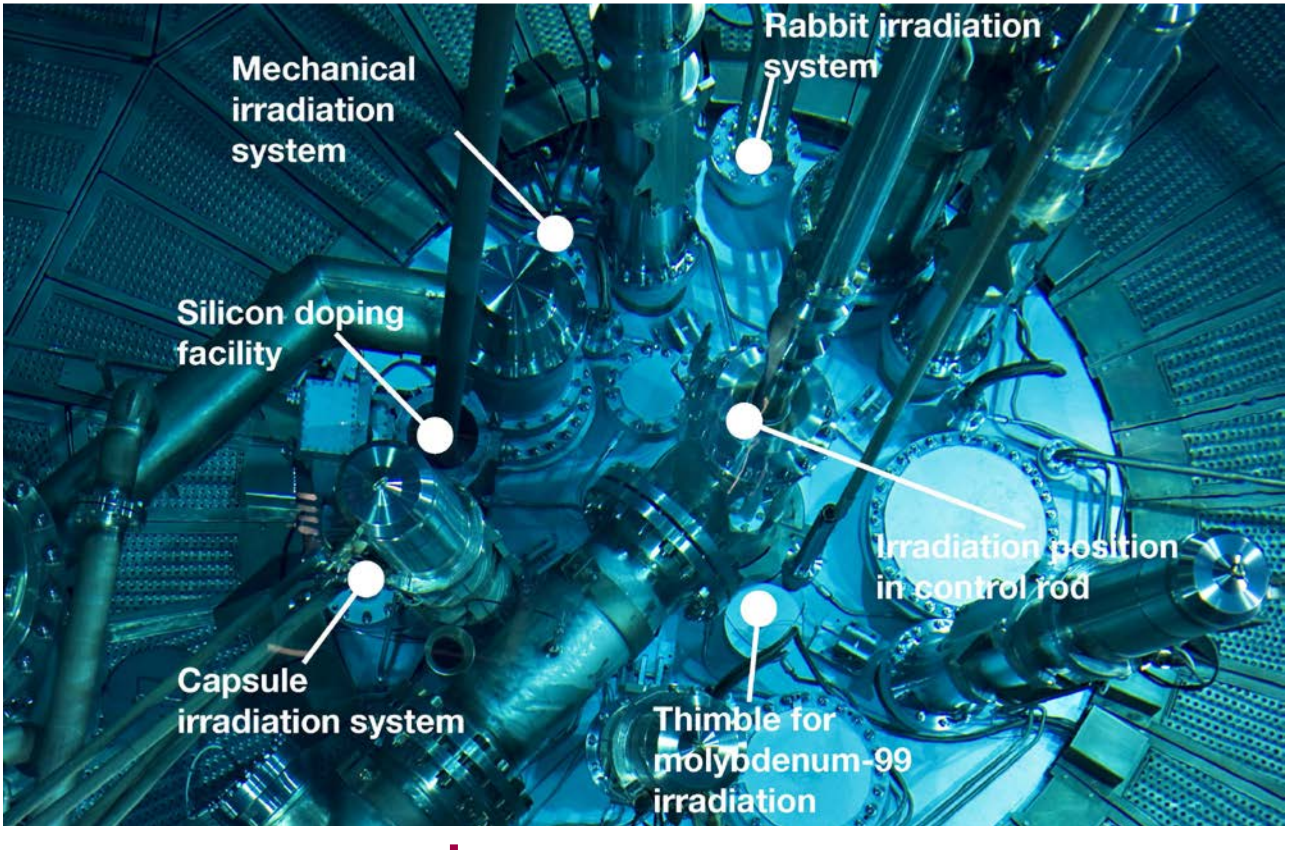
Recently, researchers from TUM contributed significantly to the understanding of a new kind of lithium-ion battery using the NDP method [1-3]. They characterised a promising new electrode candidate for silicon-graphite electrodes, however, it suffers from a loss in capacity with the number of charge-discharge cycles. Upon extended cycling the anode substantially expands in its thickness and increases in mass. The material is provided by the electrolyte, forming a so-called SEI layer ("solid electrolyte interphase"). In addition, morphological changes of the silicon nanoparticles largely increase their surface area, which further increases the SEI formation. Both results were confirmed using conventional electrochemical and imaging techniques. Using NDP, they could go one step further to discover that the increasing amount of lithium immobilised in the SEI proceeds uniformly across the thickness of the silicon-graphite electrode. The observed degradation is predominantly caused by the volume expansion/contraction of silicon nanoparticles over a charge-discharge cycles.

[1] M. Trunk et al., Materials science applications of Neutron Depth Profiling at the PGAA facility of Heinz Maier-Leibnitz Zentrum, Materials Characterization 146, 127 (2018).
[2] M. Wetjen et al., Quantifying the Distribution of Electrolyte Decomposition Products in Silicon-Graphite Electrodes by Neutron Depth Profiling, Journal of the Electrochemical Society 165 (10), A2340 (2018).
[3] M. Wetjen et al., Monitoring the Lithium Concentration across the Thickness of Silicon-Graphite Electrodes during the First (De-)Lithiation, Journal of the Electrochemical Society 166(8), A1408 (2019).

Driving innovations and industrial applications

Neutrons are a unique tool and are not only used by researchers investigating new materials at the forefront of science. They also enable industrial users to develop new products, look into process flows or produce entirely new substances, which were otherwise not available. At the FRM II we have built up additional facilities for irradiation with neutrons which do not compete with the highly requested beam days at the scientific instruments for neutron scattering. This includes a series of irradiation facilities using the high neutron flux near the reactor core for applications like silicon doping for the semiconductor industry, production of radioisotopes for nuclear medicine as well as for industry (mainly cobalt-60) or elemental analyses by means of Neutron Activation Analysis (NAA).

Using neutron methods at the scattering instruments, however, are equally well suited to answer questions in the development of commercial products or new industrial materials. Here competition between science and industry is steered by the director's board in order to offer a suitable amount of beam time for innovation in industry, thus ensuring the impact of neutrons on the daily life of people. This also includes the medical application of fast neutrons for radiation therapy. A dedicated converter facility provides these fast neutrons directly after they have been emitted from the fission of Uranium, but otherwise these neutrons are not available outside the reactor pool.



View of the reactor pool and its irradiation facilities.

Silicon doping

Our objective is to foster industrial applications. For the production of high-quality, homogeneously doped silicon for the semiconductor industry, high-flux research neutron sources, such as the FRM II, are indispensable.

Pure silicon is a very poor conductor of electricity. However, it is industrially viable for semiconductors when it contains a small amount phosphorus. The introduction of these impurities is called doping, thereby increasing the conductivity of the semiconductor material silicon in a precise way. At the research neutron source, doping is achieved using neutrons, using the so-called neutron transmutation doping (NTD) process.

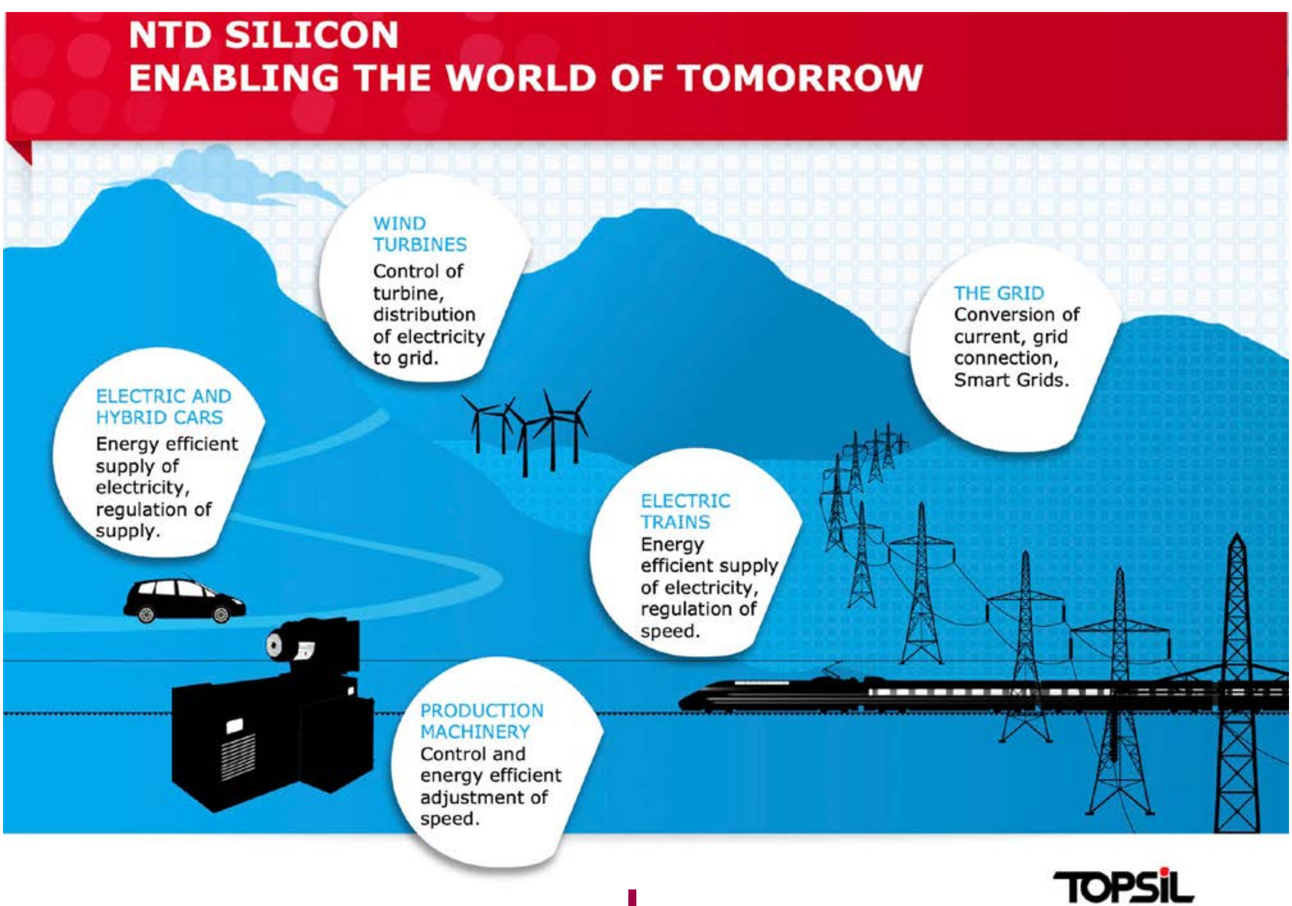
The Silicon Doping Facility at the FRM II can irradiate cylindrical Si mono-crystals, called ingots, up to 50 cm in height and up to 20 cm diameter. The monocrystalline silicon ingots are placed in a special device in the irradiation channel within the moderator tank and are exposed to a well-defined thermal neutron flux for a period of anything from a few minutes up to a full day. The neutrons transmutate individual silicon atoms into phosphorus via radioactive silicon. In contrast to other doping techniques, neutron transmutation doping used at the FRM II guarantees a particularly homogeneous phosphorus distribution in the silicon crystal and provides a uniform resistivity over a large area, producing the high-quality product desired by the customers.

Industry relies on the quality of doped silicon. Therefore, in 2011, the internal quality management system ISO 9001:2015 was introduced at FRM II. This certificate describes all procedures to be followed for the production of doped silicon as well as for radioisotope production and activation of analysis samples, Furthermore, it ensures continuous further development and improvement of the overall process, in order to meet all customer requirements. Within ISO 9001:2015, the FRM II receives feedback from the customers via a feedback management system, ensuring that any issues regarding the quality of the individual crystals are clarified and solved. All in all, the FRM II always yields very good results within the feedback management system and is always rated very well in the annual customer satisfaction evaluations in the form of a “Supplier Rating”. Up to now FRM II has always been able to maintain its position as a “Preferred Supplier”.

The demand for doped silicon by neutron irradiation is so high that at the FRM II up to 15 tons are commissioned annually by companies from Europe and Asia. The majority of orders were received from European companies. The number of silicon rods ordered by the main customers is in the three-digit range. In the period from 2012 to 2018, 5666 silicon rods were irradiated. This corresponds to an average annual output of 809 silicon rods. At the beginning of 2006, three customers were supplied; today, the number of customers has stabilised at six semiconductor producers. The amount of silicon irradiated has been increased in recent years from approximately three to approximately 15 tons of silicon. The total mass of processed silicon was 105 tons between 2006 and 2018. With a maximum annual output of 15 tonnes, the FRM II is estimated to produce up to one tenth of the world production, taking into account an estimated worldwide capacity of silicon doped with the help of neutrons of 150~180 tons per year [1]. However, the demand for high-quality and homogeneously doped silicon from research neutron sources is rising continuously.

The silicon doped by neutron transmutation is used for power semiconductor devices, including power thyristors, rectifiers as well as transistors, such as insulated-gate bipolar transistor (IGBT) and power metal-oxide semiconductor field effect transistor (power MOSFET), which all handle significant power levels. The latter are hardly used anymore due to large heat losses. Today NTD silicon is mostly used for IGBTs and thyristors. Thyristors are high-voltage, high-current semiconductor rectifiers and are required for energy transport over long distances and industrial heavy load power control. IGBTs are used in the power regulation of high-speed trains and power-efficient automotive applications.

[1] M. S. Kim et al., Estimation of future demand for neutron-transmutation-doped silicon caused by development of hybrid electric vehicle and its supply from research reactors. IEEE 13th European Conference on Power Electronics and Applications, 1-10 (2009).



Typical applications of silicon doped by neutron transmutation.

Neutron Activation Analyses for elemental composition

The FRM II offers a unique possibility for the non-destructive determination of chemical elements by means of activation analysis for industry and science. Neutron Activation Analysis (NAA) is used for the determination of heavy elements (atomic number $Z > 11$) in trace amounts, especially at the parts per million (ppm) or parts per billion (ppb) level. Here, NAA may provide both qualitatively and quantitatively fast and reliable answers. Prompt Gamma Activation Analysis (PGAA) complements this and is used to determine light elements, typically the major and minor components.

After irradiating matter with neutrons, characteristic gamma radiation is emitted which can be used for qualitative and quantitative analysis. Both neutrons and gamma rays penetrate into the sample by several centimetres; hence, all neutron-in gamma-out analytical techniques yield the average composition of the irradiated volume (bulk). The MLZ/FRM II offers the best-thermalised high-flux irradiation channels in its reactor for NAA and the strongest cold-neutron beam of the world for PGAA and in-beam NAA. A similar method using the same phenomenon, but where the energy loss of the detected particle depends on its emission depth, is the so-called Neutron Depth Profiling, NDP.

The applications of activation analyses are manifold. Using NAA, industry may look for impurities or contaminations with very low detection limits in silicon (e.g. for the semiconductor industry), plastics (e.g. toys); ceramics, steels, alloys (e.g. for high temperature turbines), electrodes of batteries or any other materials. In archaeology and cultural heritage, both, PGAA and NAA, can give useful information on the origin of prehistoric finds or identification of forgeries, based on the so-called “fingerprints” of the individual elements. Meteorites or moon rocks can also be analysed. Today, activation analyses are also widely used in life sciences and environmental monitoring, by investigating cells and tissues for their metal contents, or by investigating heavy metals in fly ash or air filters. Even for forensic purposes NAA can be applied, as was done for the famous investigation of Napoleon’s hair. NAA provided evidence that his hair had higher arsenic content than the normal level [1].

For NAA, samples are sent into the irradiation positions near the reactor core using the pneumatic rabbit irradiation system.

[1] X. Lin, R. Henkelmann, Contents of arsenic, mercury and other trace elements in Napoleon‘s hair determined by INAA using the k_0-method, Journal of Radioanalytical and Nuclear Chemistry 257, 3, 615-620 (2003).

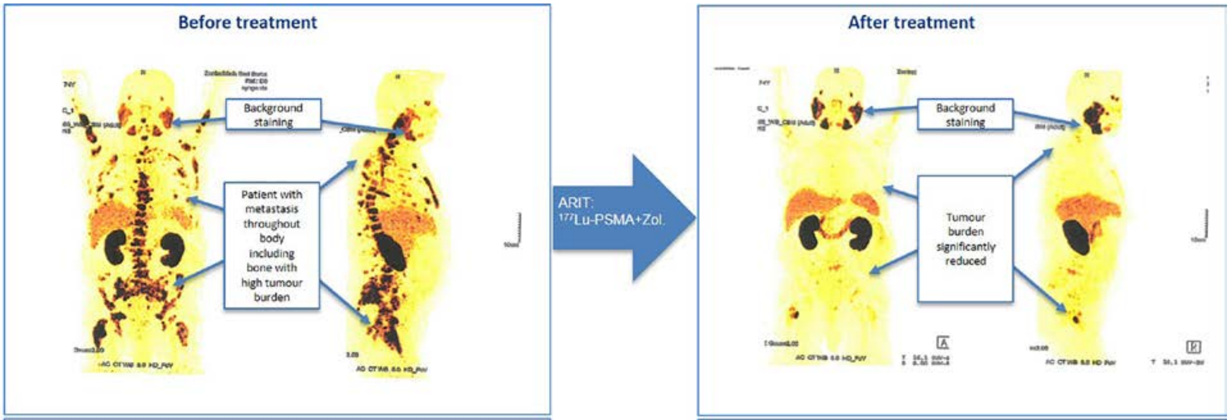
Medical applications of neutrons

The use of our neutrons for medicine is a major and utterly important application serving our society. Neutrons are indispensable for modern nuclear medicine. Radioisotopes are produced via neutron capture and are used for both diagnostics and curative purposes. The radioisotopes are produced by the neutron source and then transported to hospitals or radiopharmaceutical companies to be transformed into radiopharmaceuticals. Neutrons can also be directly used for tumour therapy, as done at the FRM II in cooperation with Klinikum rechts der Isar, representing a good palliative, and for certain tumours also a curative form of radiation therapy.

To foster the production of radioisotopes, with the support of High-Tech Offensive Bayern with in total 6.1 million €, in 2005, the Industrial User Centre (IAZ) was built on the site of the FRM II and is used by, among others, the Isotopes Technologies Garching GmbH for the production of radiopharmaceuticals, such as Lutetium-177. Having the radiopharmaceutical industry on site is a huge advantage, since it minimises the transport of irradiated and highly radioactive targets. And since medical radioisotopes usually have a very short half-life, from a few days to a few hours, it is of great advantage for the processing of the radioisotope, if neutron source and radiopharmaceutical industry are close by. The good infrastructure on the site itself, as well as proximity to the airport and its motorway connection, provides another advantage to industrial partners.

Medical radioisotopes produced at the FRM II include Lutetium-177 (Lu-177) and Holmium-166 (Ho-166) for tumour therapy and in future also Molybdenum-99/Technetium-99m (Mo-99/Tc-99m) for diagnostic purposes. Radioisotope production in that quality, purity and amount depends largely on the use of research reactors. Alternative technologies may be investigated, but cannot account for the necessary current world demand of medical radioisotopes, such as Lutetium-177 or Molydenum-99. Together with all current and future operators of irradiation facilities for the production radioisotopes, as well as all partners in industry involved in the production chain, we have to ensure the sustainable delivery of the radioisotopes, such as Mo-99/Tc-99m or Lu-177 in future years.

Industrial User Centre (IAZ) on site of the FRM II that industrial companies such as Isotopes Technologies Garching GmbH benefit from.



Prostate Cancer Patient: ^{68}Ga-PSMA PET/CT after 3 cycles of ultimately failed Chemo and Radiation Therapy

Same Prostate Cancer Patient after 2 treatment cycles with Targeted Radioisotope Therapy: ^{177}Lu-n.c.a – PSMA and Zoledrotate therapy

Case studies showing the high efficacy of targeted radioisotope therapy with Lu-177 n.c.a., using targeted PET/CT imaging.

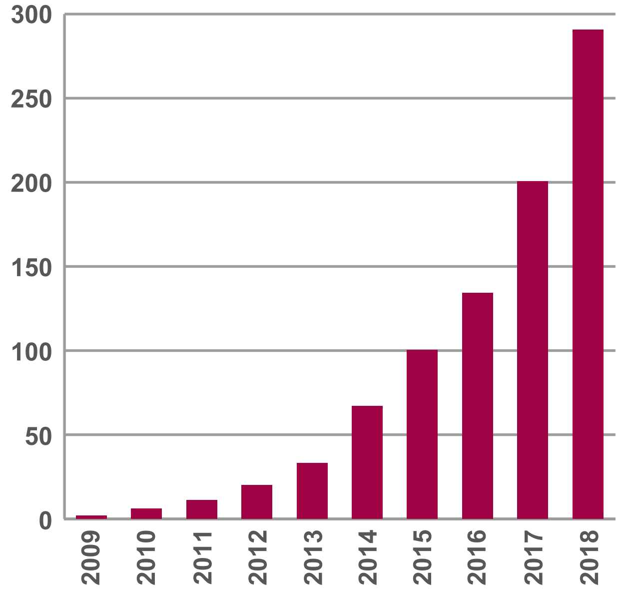
Lutetium-177

The research neutron source FRM II enables the production of no-carrier-added Lutetium-177 (Lu-177 n.c.a.). This technically very complex method was developed in 2006/2007 together with Radiochemistry Munich RCM, which is also a scientific institute based at TUM, and is utilised commercially today by the ITM Isotopic Technologies AG Munich on the site of the FRM II. Using this method at the FRM II, Lu-177 is produced from the irradiation of Ytterbium-176 (Yb-176) through a very short-lived nuclide Yb-177, which quickly decays to Lu-177. This process guarantees pure Lu-177 that is free of other stable isotopes, such as Lu-176, and is thus referred to as “carrier-free” (Lu-177 n.c.a.). This means less radioactive waste for clinics and use for a longer time since, even after 9 days, it still contains a sufficient amount of therapeutically active Lu-177.

For the Lu-177 production at FRM II the capsule irradiation facility is utilised. Four Yb-176 quartz glass ampoules with 1g Yb-176 each are irradiated between 12 and 14 days, resulting in a Lu-177 activity of 2.8 GBq at the end of irradiation. This results in approx. 1.5 GBq Lu-177 as calibrated activity for the clinics, which corresponds to approximately 220 patient doses. ITM performs four radiation units per FRM II cycle, which means approximately 900 patient doses. If the FRM II runs 4 cycles, then ITM can provide about 3,500 patient doses per year. ITM has only one irradiation position available at FRM II, but supplies a total activity of at least 7 TBq Lu-177 per week. Therefore, FRM II contributes about 12% to the total Lu-177 production of ITM. Due to the limited number of usable research neutron sources, this is a significant contribution to their Lu-177 production.

Lu-177 is used to treat so-called neuroendocrine tumours (e.g. tumours in the prostate, stomach, intestines, pancreas, and lungs). Lu-177 is in this case coupled to a peptide molecule, a so-called “ferry”, and thus moves directly into the tumour.

Figure 10: No-carrier-added Lu-177 n.c.a. and its relative growth in demand.(Data: ITM Technologies).



Lu-177 is a beta emitter (an electron and an anti-neutrino is emitted) with a very low range of about two millimetres, which means that healthy tissue remains virtually undamaged. For the therapy of prostate cancer, the radioisotope Lu-177 is coupled to the peptide PSMA within the hospitals. The success rate of Lu-177 therapy with PSMA and/or DOTATOC is well above 95%. In order to deliver the complete radiopharmaceutical product in future themselves, ITM plans to build a production site in Neufahrn by 2021/2022.

ITM went from science to industrial scale production of Lu-177 n.c.a. between 2008 and 2010. In 2011, it became a GMP-certified production process. The success story of Lu-177 n.c.a. delivered by ITM, shown by its relative increase, is depicted in Figure 10. This increasing demand and security of supply can only be covered by a reliable global reactor network, demonstrating the responsibility for the FRM II to produce this very important radioisotope.

Holmium-166

Since September 2018, the radioisotope Holmium-166 has been produced at the pneumatic irradiation facility at the FRM II for the radiation therapy “radioembolisation”. This is a novel form of treatment for primary and secondary liver tumours (i.e. liver metastases and liver cell cancer) that have proven to be inoperable or not treatable by chemotherapy.

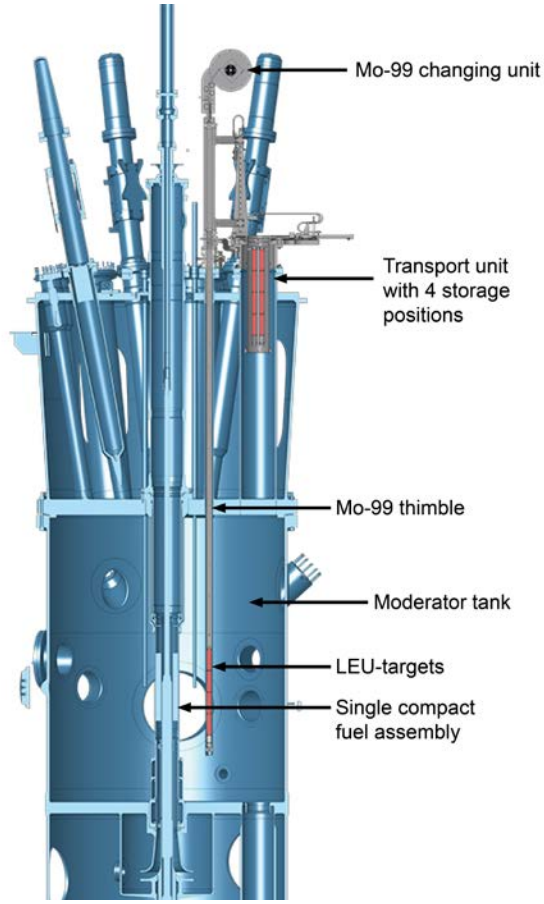
Radioembolisation is performed by injecting the fine Ho-166 beads via a microcatheter into the hepatic artery. The microspheres are transported via the bloodstream to the tumours in the liver. There they remain stuck in the capillaries of the liver, emit beta radiation and damage the tumour cells at close range, while the low-energy gamma radiation penetrates the body and can be recorded by gamma cameras. In addition, the metal holmium can be visualised in vivo by both single-photon-emission CT (SPECT) and MR imaging. Therefore, holmium-166 can be used for theranostic application by exploiting its inherent characteristics, i.e. diagnostic and therapy at the same time. The half-life of the radioactive Ho-166 is 26.8 hours, which means that more than 90% of the radiation is emitted within the first 4 days after the implantation procedure.

Molybdenum-99

The most important and most commonly used isotope in nuclear medicine is Technetium-99m, the daughter isotope of Molybdenum-99. It has a very wide application range for diagnostic purposes and usually arises as a fission bi-product of the irradiation of uranium.

Currently there are six major irradiation facilities for the production of Mo-99/Tc-99m worldwide, including four in Europe and one each in Africa and Australia. However, of these Mo-99-producing research reactors, five are already over 40 years old and three of them will stop operation before 2029. In the years 2008-2009, unforeseen, extensive and lengthy repairs were necessary in some of these reactors, which required a temporary shutdown. The absence of sufficient reserve capacity led to repeated major bottlenecks in the supply of Mo-99 between 2008 and 2010. Due to this shortage and the increasing demand of Mo-99, the FRM II decided in 2011 to install a Mo-99 irradiation facility, which will enable the production of this very important medical radioisotope Mo-99/Tc-99m. The total costs for the Mo-99 facility, currently under construction, amounts to approximately € 5.4 million and is covered by the budget of FRM II. In addition, the necessary research and development activities for the optimisation of Mo-99 irradiation were supported by the Federal Ministry of Health through a € 1.0 million contribution. The design and construction of the facility are arranged so that it will run parallel to the scientific uses of the neutron source.

The radioisotope Tc-99m is used in up to 80% of applications of in-vivo diagnostics. This corresponds to more than 30 million tests each year worldwide. In Germany alone, about 3 million tests are performed using Tc-99m. This corresponds to about one-tenth of the world's demand for Tc-99m. It is used for the investigation of thyroid function, but also for the diagnosis of diseases of other organs such as the lungs, heart, liver, gall bladder and the skeleton. The short lifetime of 6 hours of the diagnostic or therapeutic isotope Tc-99m, and the low energy of the γ-rays, minimise the exposure of the patient to radiation. Due to the transient nature of the initial isotope Mo-99 and the high demand for Mo-99/Tc-99m, Europe – and also Germany as the largest single consumer – requires its own medium and long term secured supply chain for Mo-99/Tc-99m. With a planned maximum weekly production of approximately 16,000 Curie (Ci) Mo-99 activity – (this refers to the activity immediately after the end of irradiation) – the FRM II will be able to cover up to 50% of the European future demand and will, therefore, significantly contribute to the supply security of Mo-99/Tc-99m worldwide.



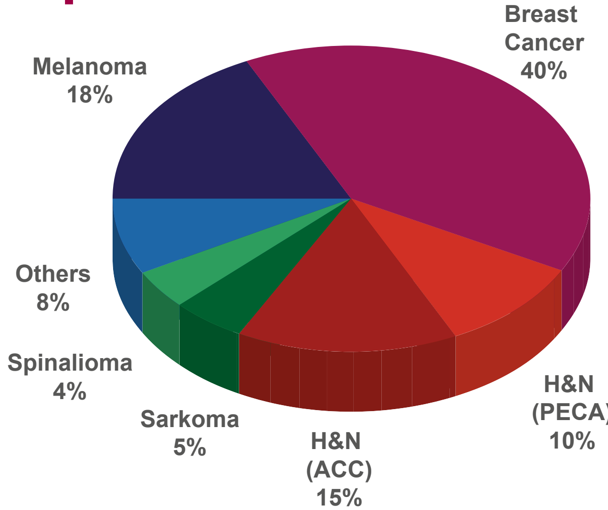
Schematic drawing of the future Mo-99 irradiation facility within the reactor pool.

Radiation therapy using fast neutrons

There are major differences between hadron radiation and the types of radiation typically available in hospitals, especially with regard to biological effectiveness and tissue penetration. Due to their energy spectrum, fast neutrons produced at FRM II have the highest relative biological effectiveness of all currently available neutron beams used in cancer treatment, comparable only to the effectiveness of heavy ion therapy. This advantage comes at the expense of penetration depth, which limits the application of fast reactor neutrons to near-surface tumours, typically mammary adenocarcinoma and melanomas (see Figure 11).

The aim of radiation therapy is to cause an irreparable break in the genetic material of the cell – the double strand of the DNA helix – and to damage it to such an extent that the cell either triggers apoptotic cell death or at least loses its ability to form colonies, a condition called clonogenic cell death. Due to their high ionisation density, fast neutrons often lead to clustered DNA damage that may exceed the cells repair capability and induce the previously named processes. The cells' own repair mechanism is absolutely vital for all living organisms, since they are exposed to natural ionising radiation from space or from the earth and to many other deteriorating influences. A healthy cell is therefore permanently engaged in DNA repair; most tumour cells are capable of this to a lesser extent, and it is this fact that healthy cells have an advantage and that side effects can be mastered.

Figure 11: Since commissioning of MEDAPP in 2007: 134 patients, about 755 irradiations of mainly near-surface tumours due to the rather low penetration depth of neutrons [1].



Fast neutrons are produced by means of a so-called converter facility in the reactor pool. Here, thermal neutrons from the reactor core hit two converter plates containing uranium-235 (U-235), and thereby induce fission processes in uranium. Fast neutrons with an average energy level of 1.9 MeV are released and travel unmoderated on a direct pathway along the SR10 beamline to the irradiation facility MEDAPP. With a flux of approximately 3.2×10^8 fast neutrons $cm^{-2}s^{-1}$, a maximum area of about 27 cm x 20 cm can be irradiated. The shape and size of the beam field can be adjusted individually to the tumour being irradiated using a multileaf collimator. The patient is positioned on the radiation table so that the tumour region marked out by the physician is covered by the neutron beam. Treatment time depends on the prescribed radiation dose; usually this is up to three minutes per field. Overall, only four to five radiation exposures per field and patient are usually necessary. The University Hospital of TUM, the "Klinikum rechts der Isar" (MRI), Department of Radiation Oncology, is responsible for conducting the therapy; FRM II only provides the irradiation.

Previously at FRM ("Atomic Egg"), a total of 715 patients underwent radiation treatment with neutrons from 1985 to 2000. At FRM II, since the commissioning of the irradiation facility in 2007, a total of 134 patients have been treated. Depending on the clinical indicators involved, neutrons represent a good palliative, and for certain tumours, such as carcinomas of the salivary gland, also a curative form of radiation therapy.

[1] H. M. Specht et al., Paving the Road for Modern Particle Therapy – What Can We Learn from the Experience Gained with Fast Neutron Therapy in Munich? Frontiers in oncology 5, 262 (2015).

The tumour irradiation facility with a face mask for precise positioning of the patient.

Contributing to industrial projects and innovation

In addition to the industrial use of our irradiation facilities, we enable innovation-driven, application-oriented research by providing access to our experimental facilities to industry. Collaborations deal, among others, with battery and electro-mobility research, irradiation tests of electronic devices, characterisation of materials, non-destructive testing of components and materials as well as the development of process engineering for industrial applications.

In the field of energy research, neutrons contribute strongly when light atoms are important or real bulk information is needed. Electro-mobility and the urgent need to store electric energy are stimulating research on lithium ion cells and the need to observe the movement of Li atoms during battery operation. In terms of energy conversion, high-temperature alloys are investigated in order to improve their mechanical properties and thus, for example, develop more efficient gas turbines with less CO_2 emission. Industry partners are increasingly aware of the unique possibilities of neutrons offering non-destructive, in-situ and in-operando studies for batteries or in-situ experiments on high-temperature alloys up to 1300°C, in combination with load or compression. Neutron Activation Analysis can determine elemental composition even in small amounts of sample material and concentrations down to ppb. With the help of more specialised methods like small angle neutron scattering, new products were developed in close collaboration with industry.

Difference between the electrode wetting at atmospheric pressure (left) and in a vacuum (right).

Filling lithium-ion cells faster

One of the most critical and time-consuming processes in battery production is the filling of lithium cells with electrolyte fluid following the placement of the electrodes in a battery cell. While the actual filling process takes only a few seconds, battery manufacturers often wait several hours to ensure the liquid is fully absorbed into the pores of the electrode stack.

The fact that neutrons are hardly absorbed by the metal battery housing makes them ideal for analysing batteries. That is why Bosch employees, in collaboration with scientists from TUM and the University of Erlangen-Nuremberg, investigated the filling process at the neutron imaging and tomography facility ANTARES.

Manufacturers of lithium cells often fill the empty cells in a vacuum. The process is monitored indirectly using resistance measurements. To make sure that all the pores of the electrodes are filled with the electrolyte, manufacturers build in large safety margins. In the light of the neutrons, the scientists recognised that in a vacuum the electrodes were wetted faster, by a factor of 2. The liquid spreads evenly in the battery cell from all four sides, from the outside in. In addition, the electrodes absorb ten percent less electrolyte under normal pressure. The culprit is gases that hinder the wetting process, as the scientists were able to demonstrate, for the first time, using the neutrons. Taking into account all parameters the filling process was performed in half of the time using the optimisation with neutron experiments.

[1] W. J. Weydanz et al., Visualization of electrolyte filling process and influence of vacuum during filling for hard case prismatic lithium ion cells by neutron imaging to optimize the production process, Journal of Power Sources 380, 126–134 (2018).

Novel paint brush cleaner works without solvents

Most paint or adhesive residue cleaners in the construction and DIY sectors consist predominantly of volatile organic solvents that release components that are harmful to the environment and health. A replacement should be found and tested that allows these harmful components to be significantly reduced or completely eliminated.

Using microemulsions instead of solvents could solve this problem. These are mixtures of aqueous and oily components as well as a large quantity of surfactants – one of them too large for practical use. Therefore, the addition of a block copolymer additive should reduce the amount of surfactant. In earlier experiments, researchers from the Forschungszentrum Jülich, together with colleagues from the University of Cologne, discovered that block copolymers could multiply the efficiency of surfactants. The block copolymers were effective but not available on the market, too expensive to produce and difficult to biodegrade.

The researchers used neutron scattering experiments at the small-angle instruments KWS-1 and KWS-2 to decipher the mode of action of the block copolymer, first in Jülich and then at the MLZ. These showed that the block copolymers were deposited at the interface between oil and water and thus reinforce the interface layer between the aqueous and oily areas of the microemulsions. This reduces the membrane area and the need for washing-active substances. They found similar properties in surfactants, which are commercially available, inexpensive and readily biodegradable.

From neutron experiment to do-it-yourself store.

The researchers also tested the desired properties of the raw materials with neutron experiments and then optimised the composition of the microemulsion. The formulation was developed in cooperation with the medium-sized company Bernd Schwegmann GmbH & Co. KG. For the first time, a colour solvent was developed that removes poorly soluble paint and varnish residues as well as soot, tar and adhesives with a small amount of surfactant and without the addition of organic solvents. The new cleaner was developed by Alfred Clouth Lackfabrik GmbH & Co. KG from Offenbach am Main and was launched on the market.

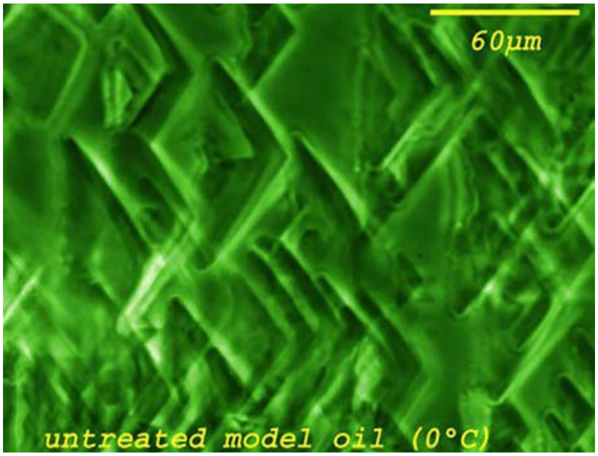
Tailored polymer additives for petrochemical products

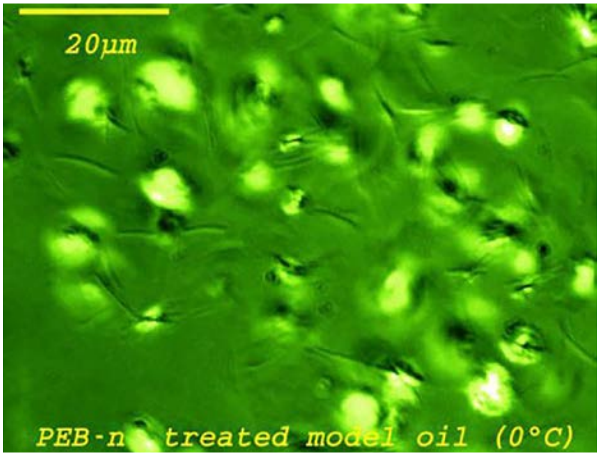
Crude oils and refined products, such as diesel fuels or heating oil, contain an important fraction of paraffins (waxes) with a broad chain length distribution. Depending on the type of crude deposits and refined technology applied, this fraction can vary between 10% and 30%. Although in terms of energy they are desirable because of their increased combustion enthalpy, they have the disadvantage of forming big crystalline aggregates at low temperatures. During the extraction of these crude oils from deep sea reservoirs, or during transport through cold regions, such fluids undergo a dramatic degradation of viscoelastic properties. A drop in temperature causes the precipitation of waxes which may plug pipelines, affect the storage tanks or clog filters of diesel motors.

To prevent this behaviour, various additives have been developed. These are polymeric systems able to moderate the wax crystals' morphology so that the oils remain fluid at low temperatures. However, the synthesis and choice of such additives is difficult. A good knowledge of the wax-polymer interaction mechanism on the microscopic scale assesses the ability of an additive to efficiently control wax crystallisation and enables the specific tailoring of the additives.

Systematic Small-angle neutron scattering (SANS) studies at the instruments KWS-2 und KWS-3 on specific polymers have provided information used, in part, for the formulation of the diesel fuel additives Paraflow™ (Infinium, Ltd.). Further extensive SANS studies demonstrated that polymeric systems exhibiting graded crystallinity along the chain may represent optimally efficient and versatile additives for waxy crude oils and petrochemical products [1]. Specifically designed polymers are able to control the wax crystallisation in medium-sized soft aggregates, thus arresting the growth of large compact waxy crystals and preventing wax gelation.

[1] A. Radulescu et al., Tailored Polymer Additives for Wax (Paraffin) Crystal Control, in Crude Oil Emulsions – Composition Stability and Characterization, Ed. M. Abdel-Raouf, IntechOpen, 205-230 (2012).



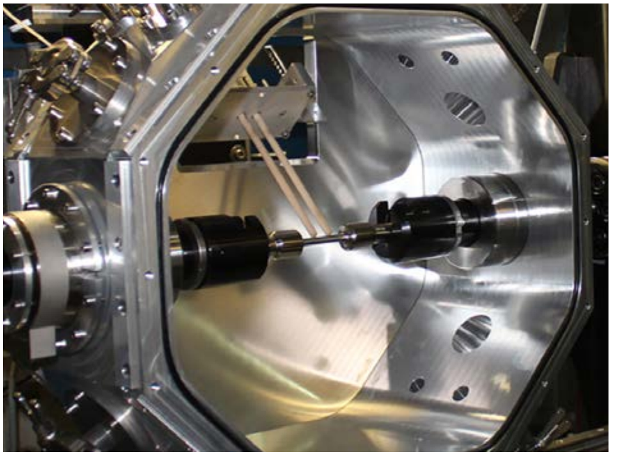


Wax gelation in crude oils at low temperatures (top). Crude oils remain fluid after addition of specifically designed polymers (bottom).

The innovative testing machine for in-situ neutron experiments

In the field of high-temperature alloy applications gas turbines play a significant role in terms of energy conversion. In particular, the stepwise improvements of Ni-based superalloys from wrought to cast alloys with excellent properties as high-temperature strength or corrosion and creep resistance including high fracture toughness are in focus. The main goal of existing Ni-base superalloys is to increase the operation temperature of these alloys in gas turbines to allow engine manufacturers to improve the fuel efficiency and therefore have a positive effect on the environment. All the superalloys consist of γ´ precipitates coherently embedded in a γ matrix plus additional high-temperature phases (e.g. δ and/or η). Over the last few decades the scientific community has put great effort into the development of Ni-based alloys for stationary gas turbines with operation temperatures above 650°C, whilst keeping the good processing characteristics of the well-known alloy 718.

In order to test new superalloy candidates, TUM is developing an innovative testing machine in the frame of a BMBF project. Together with VDM Metals and TU Braunschweig the alloys will be studied with neutrons. The testing machine will be set up at the instrument STRESS-SPEC providing loading (up to 100 kN) and compression experiments and temperatures up to 1,200°C. Furthermore, a feature for quenching the sample is implemented to simulate the performed heat treatment and cooling of the industrial manufacturing process. An extension for cracking characterisation is foreseen, too. The new testing machine will facilitate, among other different measurements, the simulation of the



Testing machine in operation at the instrument STRESS-SPEC.

forging process at high temperature of this type of material by compressive tests and the gained understanding can be directly translated into important industrial alloy development.

[1] C. Solís, et al., In-situ characterization at high temperature of VDM alloy 780 Premium to determine solvus temperatures and phase transformations using neutron diffraction and small-angle neutron scattering, Characterization of Minerals, Metals, and Materials, TMS 2019, Conference Proceedings (2019).

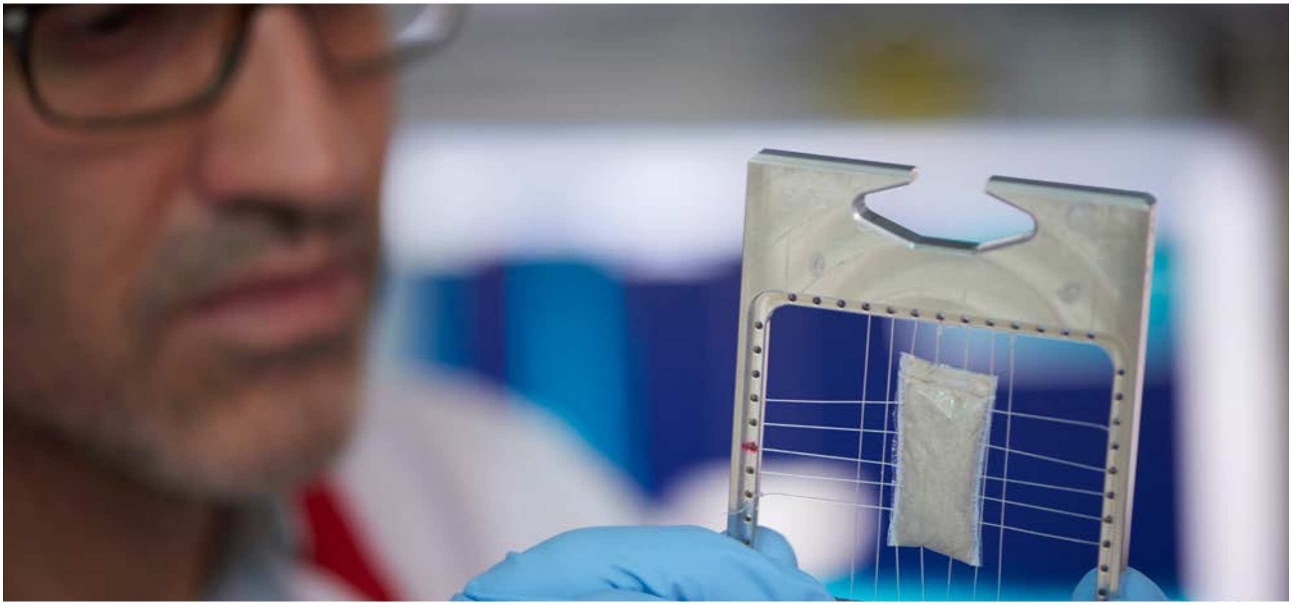
[2] C. Solís, et al., In situ characterization at elevated temperatures of a new Ni-based superalloy VDM-780 Premium, Metallurgical and Materials Transactions A 49, 4373-4381 (2018).

Boron equivalent as a measure of impurities

Graphite is used in industry in large quantities, for example as electrode material for batteries, for filtering purposes and in nuclear plants as reflector and moderator material. Technical graphite usually contains impurities with other elements such as chromium, iron, nickel, manganese, lead and boron, which severely restrict its use. In the case of graphite, which is used in nuclear facilities, the contamination with boron is particularly disturbing due to the high absorption cross section for thermal neutrons.

The trade in nuclear materials is strictly controlled internationally. Graphite may therefore only be exported as “nuclear pure” graphite and with special conditions. Nuclear pure graphite is graphite with a degree of purity corresponding to a so-called boron equivalent of less than 5 ppm and with a density of more than 1.50 g/cm^3. An exact determination of the boron equivalent is therefore important for many industrial applications, sometimes even regulated by law. Both neutron activation analysis (NAA) and prompt gamma activation analysis (PGAA) can be used for this purpose.

The FRM II has a number of irradiation channels for neutron activation and enables multi-element analysis by combining NAA and PGAA. The PGAA is best suited for boron equivalent determination because the method is based on the measurement of the elements with the largest cross sections for neutrons. The NAA allows accurate measurement of all trace elements, but is no longer accurate enough for light elements such as boron, hydrogen and nitrogen. However these elements make the highest contribution to the boron equivalent. The customer therefore gets a very comprehensive result with a PGAA analysis, selected according to elements.



Prompt Gamma Activation Analysis finds impurities in materials.

Educating high professionals and public engagement

Being part of the Technical University of Munich, there is no discussion on whether we have to educate students or not. As a research facility offering powerful but complex methods we have a strong interest of our own to train our users as future potential customers. The education of students in Bachelor, Masters or PhD studies is manifold. Well educated students will rely and use neutron methods whenever it is advantageous for their research topic during an academic or scientific career. On the other hand, as most of the scientists will work in industry later, this spreads the knowledge of neutron methods to a broad area of applications. Education and training of high professionals in general has a strong impact on society, especially addressing the grand challenges of today, and thus it is an inherent part of our mission.

Our activities and achievements would be less effective or would perform a lower impact on society if we do not communicate our findings and developments. This communication naturally has a strong focus on our existing or potential users. The communication to the general public, however, is equally important as research funded by public money relies on a broad acceptance by our society. This communication is very effective on site in Garching where visits of interested groups are organised on a nearly daily basis. Modern communication in social media, internet pages or press releases complement our engagement.

Education and training

Education has always been a key mission for the FRM II and the MLZ. This mission is inherently related to the uniqueness of neutron research, but also limited within university courses as practical training is not possible without a neutron source. By the end of 2019, besides the FRM II, the small research reactor at the university in Mainz are the only neutron sources available in Germany. The engagement in practical courses at our instruments, however, has to be balanced alongside the available beam days for our scientific and industrial users. To address complicated research programs, the choice of methods applied usually comprises a selection of different experimental techniques. Neutron research has to compete and complement other techniques, which is one of the reasons that we welcome an increasing number of non-expert users at our facility. MLZ is counteracting this with a dedicated educational program, ranging from lectures and lab courses, to supervision of bachelor/ masters/ PhD theses, to dissemination of information at conferences or other events to promote the usage of neutrons.

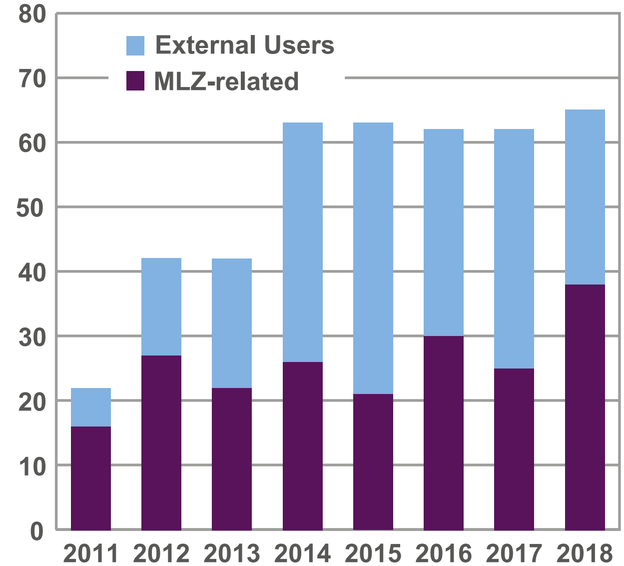
Being located at the heart of a still-growing science campus based on TUM's science and engineering faculties, and including the connections of the MLZ partners to their home universities throughout Germany, ensure a strong impact on education. As the profound understanding of neutron scattering requires a solid basis in solid state physics and quantum mechanics, teaching starts primarily at masters level, but it has also been possible to capture the enthusiasm of students at earlier stages in their academic career.

The established way of educating students in neutron scattering consists of a series of lectures. Courses dealing with the general and specific aspects of physics with neutrons are part of the bachelor and masters curricula at TUM. Just to name two examples, "Physics with Neutrons" deals with the entire topic of thermal neutron scattering while "Reactor Physics" is more concerned with nuclear technology and the operation of the neutron source itself. Furthermore, all MLZ partners give lectures at their respective home universities.

In addition to lecture cycles, MLZ also offers university lab courses. About 1/3 of all physics students at TUM perform practicals on MLZ instruments; these lab courses are also part of the TUM Materials Sciences master's degree in Mechanical Engineering. Through cooperation with JCNS, the University of Paderborn also performs an annual lab course at the MLZ. These lab courses are often the students' first contact with neutron scattering and large scale research facilities, and regularly these students stay on in trainee positions after the course has concluded.

Neutron schools offer students and postdocs the opportunity to learn the essentials of neutron scattering in theory and practice.

Figure 13: Completed PhD Theses using experimental facilites at the MLZ [1].



In order to educate students and postdocs who did not have the opportunity to attend a neutron scattering lecture or lab course at their university, MLZ partners have organised a variety of neutron schools that cater for different interests. JCNS organises the well-established Neutron Laboratory Course every summer, which is divided into one week of lectures in Jülich and a one week practical course using MLZ instruments. Typically about 150 students apply for the laboratory course, of which 55 are selected. GEMS and MLZ organise the MATRAC school "Application of Neutrons and Synchrotron Radiation in Engineering Materials Science", which provides a systematic overview on the application of neutrons and synchrotron radiation for the structural and dynamical analysis of materials.

MLZ staff act as advisors and supervisors in Bachelor, Masters, and Doctoral theses, leading their protégés to degrees at the Technical University of Munich, RWTH Aachen and many others. Furthermore, the MLZ attracts numerous groups and external users to perform experiments using neutrons and positrons for bachelor, masters/diploma and PhD theses. In natural sciences, the first real qualifying degree is usually the Masters degree, therefore Figure 12 and Figure 13 show the Masters and PhD theses completed between 2011 to 2018, respectively. Theses that are MLZ-related are shown in dark colour, the recorded ones from external users are depicted in light colour. For the latter, regular user surveys are conducted but the theses counted may not reflect a complete list of all students having used MLZ data in their theses.

The number of finalised Masters and Diploma theses has been stable over the years (Figure 12). In addition to the master's students directly hosted by one of the MLZ partners or a user group, there has been a steady influx of master's students from a trans-European course: "Master in Materials Science Exploiting Large scale Facilities" (MaMaSELF). This is part of the ERASMUS programme

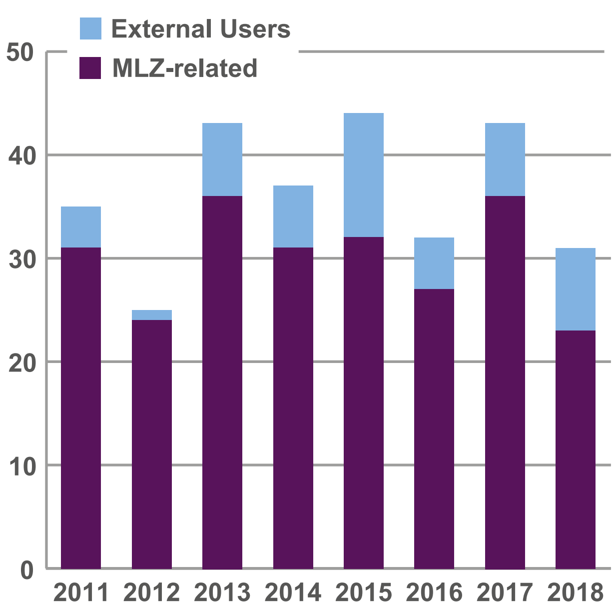


Figure 12: Completed Masters/ Diploma Theses using experimental facilites at the MLZ [1].

and connects universities in Germany, France and Italy with large scale neutron or synchrotron facilities in Germany, France, Italy, and Switzerland. The numbers of PhD graduates rose considerably, to an average of more than 60 per year (Figure 13). The majority of these are affiliated to user groups. About 70% of all PhD students were based in Germany, about 24% elsewhere in Europe and 6% came from the rest of the world.

In 2014, the TUM Graduate School (TUM-GS) programme was initiated, which became mandatory for doctoral students at TUM. Faculty Graduate Centres and interdisciplinary Thematic Graduate Centres at TUM aim to enhance knowledge transfer and collaboration to support doctoral students in their research work. Additional courses are offered on professional and soft skills to prepare students for leading positions in science, industry and society as a whole. To train and promote the exchange and community of students who are permanently based at the MLZ, special training on neutron research will be offered in the framework of a future MLZ Doctoral School.

These numbers and efforts demonstrate that the MLZ plays a significant role in the education of highly qualified future scientists. In addition, education in neutron sciences at university level is a key issue for the future development of MLZ's user base. Therefore, Forschungszentrum Jülich GmbH and TUM have agreed to create a joint professorship between JCNS and the Physics Department, hosted by MLZ.

Further efforts in education already starts by offering positions for apprentices. The FRM II/MLZ offers apprenticeships in different areas, including mechatronics, systems integration and software

Degree Awarding Ceremony of MaMaSELF graduates at the Université de Rennes 1 in September 2019.

application. Last year, one of our supervisors, Jens Krüger, was awarded the Augus Föppl Medal for his outstanding success in teaching young people. Up to now, 46 apprentices have got their education and training in different areas at the FRM II and usually graduate with best marks.

[1] MLZ publication archive iMPULSE, 2019-04-04 and data from regularly conducted user survey.

Dissemination

Telling the success stories and creating awareness and interest is our main concern, with a view to attracting new users and keeping existing ones informed. The main dissemination channel for scientific results comprises of publications in scientific journals and theses. The MLZ also organises a number of dissemination events that often serve to promote scientific results obtained using neutrons as well as to acquire new users for the facility. The events can be grouped by target audience, ranging from neutron scattering experts to scientists and engineers in academia and industry who have little or no experience with this technique.

For neutron scattering experts, the MLZ aims to be a platform for high quality intellectual exchange, simultaneously positioning itself as a world leading centre for neutron science and fostering dialogue between users and instrument scientists. The most prominent examples for these activities are probably the annual MLZ conferences “Neutrons for ...” (“Neutrons for Energy” in 2016, “Neutrons for Health” in 2017, “Neutrons for Culture and Arts” in 2018, “Neutrons for Information and Quantum Technologies” in 2019) and the JCNS workshops with alternating subjects, covering soft matter/biophysics, magnetism/quantum phenomena, and instrument/method development. The numerous small workshops on specific topics of data evaluation, specific techniques, or the possible future instrument suite at the PIK reactor in Gatchina also fall into this category. Of course, MLZ is also present on the international, European and the German neutron scattering conference, the latter event being hosted by GEMS in collaboration with the Christian-Albrechts-Universität zu Kiel in 2016.

There are also dedicated workshops organised around specific academic fields, such as energy, health and archaeology. The latter include topical workshops about non-destructive investigations for archaeologists and curators from museums dealing with heritage objects. The so-called VDI (Verein Deutscher Ingenieure) TUM Expert Forum established in 2004 is a biannual event with about 80 participants providing an excellent platform for

MLZ Conference: Neutrons for Information and Quantum Technologies in June 2019 in Lenggries, Germany.

In 2018 we celebrated 10 years of our Newsletter.

industry networking, enabling direct exchange with industry to discuss or even solve their open questions and to foster new industrial collaborations. All these workshops are held with the express aim of acquiring new user communities in science and industry.

An even wider audience is reached at the annual spring meeting of the condensed matter section of the German Physical Society, the largest annual physics conference in Europe. The MLZ has been present at these conferences by organising ”focus sessions” and having a booth in the general area, where a large number of people can and do inform themselves about the possibilities of neutron scattering in general and the MLZ facilities in particular. Operated by the Public Relations group, targeted information is provided through three different Web-Sites. Informing our users about the possible application of neutrons and positrons, as well as information from the user office on how to access the instruments of the MLZ, is given by the MLZ web-page under mlz-garching.de. Information for the general public, especially on the operation of the nuclear facility FRM II and its use for research, industry and medicine is given separately under frm2.tum.de. In addition, the MLZ operates the international web page neutronsources.org, where information from all neutron sources is gathered and international events are promoted.

Furthermore, information is actively provided by using our social media channels, such as facebook and twitter, and also by target-oriented brochures, leaflets and newsletters.

6th VDI-TUM Experts Forum in September 2016 in Garching, Germany.

A walk-in model of the Atomic Egg featuring original MLZ sounds makes exhibitions on neutron scattering a much more immersive experience.

Public outreach

Communication with the public is very important for the FRM II/MLZ. The usual way to do this is via the media newspapers, magazines, radio and TV, which is primarily organised through press releases. These tend to have a large audience, as MLZ press releases are also distributed by the press offices of TUM and Forschungszentrum Jülich GmbH. Additionally, there are also channels where MLZ can distribute information more directly to its audience, such as its website and social media channels, as well as facebook and twitter, self-produced print products, and videos on YouTube. The news feed “FRoM behind the SCiENcES” is supplemented with more personal aspects about people working at the FRM II/MLZ in order to establish an emotional connection with the public. Importantly, this indirect channel is supplemented by personal contact. MLZ follows a two pronged approach: MLZ employees interacting with the public off-site, and opening the doors of the facility on-site.

MLZ scientists’ off-site interaction with the public primarily consists of scientific talks in a variety of settings. Some of these have even be televised in the frame of the “ARD-alpha Campus TALKS” series on German national TV. Most notably, MLZ contributes to both the lecture series “Wissenschaft für Jedermann” at the Deutsches Museum in Munich city centre and the annual “Edgar-Lüscher-Seminar”, which is organised in collaboration with the TUM Physics Department. “Wissenschaft für Jedermann” is aimed at the general public, while at the “Edgar-Lüscher-Seminar” high school physics teachers learn about the latest developments in different scientific fields connected to MLZ and can transport the knowledge and enthusiasm into their schools.

Contact with people without previous scientific knowledge and interests is very important. There has always been an MLZ contribution to the local trade fair in Garching, and this audience has recently been targeted more specifically by including art in the communication. Art exhibitions (paintings and photographs) were installed at the underground station in Garching and in a museum and an art gallery in Munich. TUM architecture students have even built a human sized model of the Atomic Egg featuring real sounds from the facility, which has attracted a lot of attention. Furthermore, we regularly take part at scientific and public events, such as the Streetlife Festival in Munich and the “Highlights of Physics” science festival in different cities of Germany with a nationwide audience as well as the Science in the City Festivals in different European cities every two years with a broad international audience.

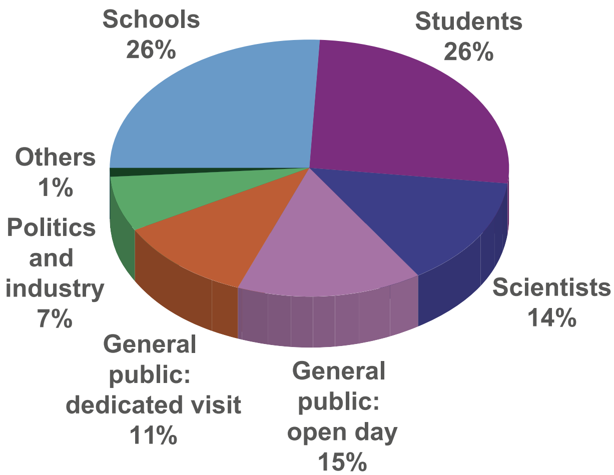


Figure 14: Categories and distribution of about 3300 visitors annually at the FRM II/MLZ in the years 2014-2017.

We aim to inspire even very young people to take an interest in the natural sciences. Therefore, we offer special programs for kids and tours on the so-called National Girls' day and we also open the doors on the so-called "Mouse day" or "Türöffner-Tag" initiated by the team of the famous German children´s programme „Sendung mit der Maus".

A steady influx of people visit the reactor: school student internships, taster courses in the school holidays; short peeks into the reactor and the instruments operated here during reactor tours, organised by the visitor's service and held by MLZ staff; or the day of open doors/long night of science. These tours of the facility are open to the public, however numerous scientific visitors attend them as well (see Figure 14). From 2014 to 2017, on average about 3,300 persons per year took part in a guided tour.

The MLZ's outreach activities are also broadly acknowledged within the field; MLZ helps organise the PARI workshops on "Public Awareness of Research Infrastructures Communicating the Importance of Science to Society" where science communications experts from all over Europe gather in order to exchange best practices and latest ideas. The first two events were held in Garching.

Showing our younger visitors how to make ice cream with very low temperatures during the „Mouse day" at the MLZ.

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